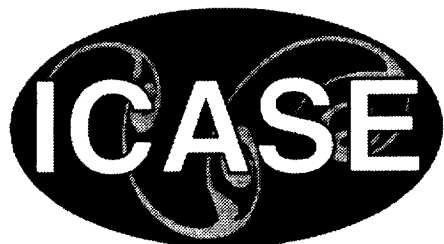


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## **Semiannual Report**

*October 1, 1998 through March 31, 1999*

*Institute for Computer Applications in Science and Engineering  
NASA Langley Research Center  
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## INTRODUCTION

The Institute for Computer Applications in Science and Engineering (ICASE)\* is operated at the Langley Research Center (LaRC) of NASA by the Universities Space Research Association (USRA) under a contract with the Center. USRA is a nonprofit consortium of major U. S. colleges and universities.

The Institute conducts unclassified basic research in applied mathematics, numerical analysis and algorithm development, fluid mechanics, and computer science in order to extend and improve problem-solving capabilities in science and engineering, particularly in the areas of aeronautics and space research.

ICASE has a small permanent staff. Research is conducted primarily by visiting scientists from universities and industry who have resident appointments for limited periods of time as well as by visiting and resident consultants. Members of NASA's research staff may also be residents at ICASE for limited periods.

The major categories of the current ICASE research program are:

- Applied and numerical mathematics, including multidisciplinary design optimization;
- Theoretical and computational research in fluid mechanics in selected areas of interest to LaRC, such as transition, turbulence, flow control, and acoustics; and
- Applied computer science: system software, systems engineering, and parallel algorithms.

ICASE reports are primarily considered to be preprints of manuscripts that have been submitted to appropriate research journals or that are to appear in conference proceedings. A list of these reports for the period October 1, 1998 through March 31, 1999 is given in the Reports and Abstracts section which follows a brief description of the research in progress.

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# RESEARCH IN PROGRESS

## APPLIED AND NUMERICAL MATHEMATICS

### BRIAN ALLAN

#### *Closed-loop Separation Control Using Oscillatory Flow Excitation*

Experimental results have shown that oscillatory blowing, introduced upstream of a separated boundary layer, can effectively delay boundary layer separation. This method for separation control can be used for several different flow control problems. Some of the current research areas of separation control are high lift enhancement and maneuver control. This project will develop a feedback controller which will control the amount of separation in the boundary layer. The feedback controller designed will then be used in a wind tunnel test on an airfoil model with oscillatory blowing.

Currently we have a design methodology for the feedback controller using a robust control design method. The controller is designed to track a desired pressure gradient in the separated boundary layer. We will not know what the dynamics of the flow system are until the wind tunnel tests are conducted. When the wind tunnel tests start, we will be able to get an accurate model of the system. This model will then be used in our current controller design methodology. We are also building a hardware interface for the flow experiment which will provide the feedback control to the experiment. This hardware interface is designed to be transferable to other flow control experiments at NASA Langley.

This control design method and hardware interface are scheduled to be tested on a future wind tunnel test. The hardware interface and control design experience gained from this project, will be transferred to other flow control experiments at NASA Langley.

This research was conducted in collaboration with Jer-Nan Juang (NASA Langley), David Raney (NASA Langley), and Avi Seifert (NRC).

### EYAL ARIAN

#### *Approximations of the Newton Step for Large-scale Optimization Problems*

Quasi-Newton methods for large-scale optimization problems are powerful but suffer an initial slow convergence rate. Our goal is to develop a new iterative method, for the solution of large-scale optimization problems, that will allow a better approximation for the Newton step right from the first optimization steps.

In the course of the optimization process, systems of linear equations are constructed that contain the linearized state operator and its adjoint. These have to be solved at each iteration to achieve convergence of the iterates to the Newton step. We are investigating a defect-correction method to solve these systems of equations for highly ill-conditioned problems with many design variables. Preliminary numerical tests on the potential small disturbance shape optimization problem are promising.

Our plan is to further investigate the above method for applications that are governed by nonlinear equations. This approach can be naturally embedded in a SQP formulation of the problem.

This research was conducted in collaboration with A. Battermann and E. Sachs (Universität Trier, Germany).

### *Large-scale Aerodynamic Shape Optimization*

The purpose of this work is to develop and apply algorithms which do not require more than a few full solutions of the flow equations to obtain the optimum.

Our approach is to apply approximations in the PDE level to the numerical solution of a practical large-scale optimization problem. We are working on shape optimization of a 3D geometry using TLNS3D.

This research was conducted in collaboration with V. Vatsa (NASA Langley).

### **H.T. BANKS**

#### *Electromagnetic Interrogation of Structures*

The detection and characterization of subsurface damage (cracks, internal corrosions, etc.) is an important problem in aging structures such as airfoils, etc. In collaboration with scientists in the Nondestructive Evaluation Branch at NASA, we are developing computational techniques for inverse problems involving electromagnetic interrogation of structures using superconducting quantum interference devices (SQUIDS).

Our approach is to develop reduced-order model computational methods for Maxwell's equations in a dielectric medium to be used in inverse algorithms. To date, we have developed models based on eddy current interrogation of structures. These models are being tested using a full Maxwell solver in ANSOFT which computes time-dependent fields in terms of a vector magnetic potential  $A$  in phaser form. Our reduced-order methods are based on Karhunen-Loeve or Proper Orthogonal Decomposition (POD) methods.

We have made significant progress on the modeling and computational aspects of this problem and are currently testing our ideas with simulated SQUID data for model verification and assessment of the ability to identify and characterize damage geometries in a structure.

### **BORIS DISKIN**

#### *Efficient Methods for Solving Upwind-biased Discretizations of Advection Equation*

The efficiency of methods for solving the advection equation is extremely important in devising solvers for complicated computational fluid dynamics problems. Frequently, the overall convergence rate of a sophisticated solver is determined by the convergence in a build-in algorithm solving the advection equation. The simplest way to solve the advection operator is to employ downstream marching. If the corresponding discretization is a stable upwind discretization and the field of velocities does not recirculate, then this marching proves to be a very efficient solver yielding an accurate solution to a discretized nonlinear advection equation in just a few sweeps (a single downstream sweep provides the exact solution to a linearized problem). However, if a discretization of the advection operator is not fully upwind (e.g., only upwind-biased) then marching in its pure form is inapplicable and other solution methods should be employed. In this period, we systematically studied two methods for solving upwind-biased discretizations of the advection operator: the defect-correction method and the multigrid method using semicoarsening. This research was motivated by the search for an explanation of convergence properties of an existing full Euler system solver and also by the wish to extend the range of available advection solvers taking into account parallelization perspectives.

The defect-correction and multigrid methods have been analyzed in application to discretized advection equations corresponding to flow at some angle of attack to a uniform Cartesian grid. We have developed a novel comprehensive mode analysis. This analysis predicts the convergence rate for each iteration and the asymptotic convergence rate. On the base of this analysis, we have explained many surprising details observed

in numerical calculations (e.g., establishment of a good asymptotic convergence rate after many poorly converging defect-correction iterations and fast convergence in a multigrid cycle employing semicoarsening far surpassing the theoretical limit predicted for standard multigrid algorithms using full coarsening). It has been found, analytically and experimentally, that the convergence properties of the defect-correction iterations are grid-dependent. The number of iterations required to converge algebraic error below the truncation error level might grow on fine grids as a negative power of the mesh size. On the contrary, the efficiency of the multigrid algorithm does not deteriorate with increasing the cycle depth (number of levels) and/or refining the target-grid mesh. This multigrid method uses colored relaxation schemes on all the grids and, therefore, is very attractive for parallel computing. A new very efficient adaptive multilevel approach to deriving a discrete solution approximating the true continuous solution within a given relative accuracy is developed. This approach was tested for both the defect-correction and multigrid methods.

As an additional option, we are going to analyze the predictor-corrector method for solving upwind-biased discretizations. We also plan to implement some of the proposed ideas in the framework of the existing 3D full Euler system solver.

This research was conducted in collaboration with J.L. Thomas (NASA Langley).

## JAN S. HESTHAVEN

### *Well-posed Perfectly Matched Layers for Advective Acoustics*

The ability to simulate accurate wave phenomena is important in several physical fields, e.g., electromagnetics, ambient acoustics, advective acoustics associated with a mean flow, elasticity, and seismology.

Often the numerical simulations of such problems, due to limited computing resources, must be confined to truncated domains much smaller than the physical space over which the wave phenomena takes place. In such cases, numerical reflections of outgoing waves from the boundaries of the numerical domain can falsify the computational results. This artifact limits the overall order of accuracy of the algorithm used in the computation. This is particularly troublesome in cases where higher-order of accuracy is required by mode resolution, storage availability, etc.

Utilizing a mathematical framework created for the development of perfectly matched layer (PML) schemes within computational electromagnetics, we have developed a set of strongly well-posed PML equations for the absorption of acoustic and vorticity waves in two-dimensional convective acoustics under the assumption of a spatially constant mean flow.

A central piece in this formulation is the development of a variable transformation that conserves the dispersion relation of the physical space equations. The PML equations are given for layers being perpendicular to the direction of the mean flow as well as for layers aligned parallel to the mean flow.

The efficacy of the PML scheme has been tested by solving the equations of acoustics using a fourth-order scheme, confirming the accuracy as well as stability of the proposed schemes.

The development of a PML for the three-dimensional equations of acoustics is straightforward provided only that the mean flow can be considered spatially constant. Of equal importance, however, is the development of PML methods for problems involving smoothly varying mean flows, as in boundary layers and jets. While the mathematical tools developed so far certainly are applicable for sufficiently smooth variations, new developments are most likely needed to address the general variable coefficient problem and we hope to address these questions in the near future.

This research was conducted in collaboration with S. Abarbanel (Tel Aviv University) and D. Gottlieb (Brown University).

## MICHAEL LEWIS

### *Pattern Search Methods for Nonlinear Optimization*

Pattern search methods for nonlinear optimization have a number of features that make them attractive for use in engineering optimization. These methods are easy to understand and implement, are scalably parallel, and neither require nor estimate derivatives.

We have developed pattern search algorithms for general nonlinearly constrained optimization guaranteed to possess first-order stationary point convergence. We are presently engaged in an implementation of the new classes of pattern search algorithms. This new implementation will allow us to investigate various algorithmic approaches, as well as opportunities for improved computational parallelism.

Among the algorithmic approaches we will investigate are techniques to improve scaling in pattern search algorithms via the aggregation of similarly scaled design variables. We will also investigate opportunities for algorithmic steering in connection with pattern search algorithms.

### *A Posteriori Finite Element Bounds for Sensitivity Calculations*

In the optimization of systems governed by differential equations one would like to use the coarsest mesh possible at any given step so as to reduce the cost of the optimization iteration. In a recent series of papers, Patera, Peraire, and their collaborators have presented an *a posteriori* approach to computing *quantitative* bounds on the mesh dependence of certain functionals of the solutions of differential equations. We have begun to apply these ideas in the context of optimization.

We have developed *a posteriori* bounds for sensitivities of output linear functionals with respect to various parameters (such as coefficients) in boundary-value problems. Using either the sensitivity equations or adjoint equations one can write the output's sensitivity as a functional of the solution of a system of differential equations. One then computes bounds on the error in the sensitivities on a coarse grid relative to a finer grid. Numerical results indicate that the bounds can be quite good. We have also extended the *a posteriori* bound approach to certain non-smooth functionals.

We are currently investigating extensions of the bound procedure to more complex equations and output functionals. We are also implementing an approach to using the *a posteriori* bound procedure in connection with pattern search methods, a first step in a larger investigation of using approximate function values with error bounds in optimization.

This research was conducted in collaboration with Tony Patera and Jaime Peraire (Massachusetts Institute of Technology).

### *Analysis of Hessians in Parameter Estimation Problems Governed by Differential Equations*

Parameter estimation problems in systems governed by differential equations arise frequently in non-destructive evaluation and materials characterization. Similar problems also arise in design optimization. In both cases it is useful to understand the analytical nature of the resulting optimization problems.

We have completed a preliminary study of the Hessians of the objective for a class of optimization problems that arise in design and in parameter estimation. We have established how, in many instances, the Gauss-Newton approximation of the Hessian may prove to be very much in error when compared to the complete Hessian.

Future work includes extending the analytical approach to more complex equations, and further investigation of the consequences of this analysis for numerical computation, particularly for quasi-Newton updates and preconditioning.



## JOSIP LONČARIĆ

### *Spatial Structure of Optimal Flow Control*

Designing distributed control systems begins with the sensor/actuator placement problem. While in some situations discrete search of combinatorial complexity seems unavoidable, continuum problems suggest solving a related question. *If one could sense everything and actuate everywhere, what should one do?* The answer to this question has polynomial complexity (of order  $N^3$  where  $N$  is the number of state variables) and can serve as the initial effectiveness filter capable of rejecting a large portion of the design search space. This favorable situation can have several causes depending on the base flow pattern. Our aim is to develop efficient numerical procedures to solve this problem for flows in moderate Reynolds number regimes.

In an earlier work, we developed a rational approximation of the optimal feedback kernel for unsteady Stokes flow. For the flow around a cylinder, this approximation was proven to perform within 0.026% of the exact optimum even in the worst case. Using the vorticity representation in conformally mapped geometries, this approximation is decomposed into the analytic free space solution and a boundary term which can be evaluated numerically. This procedure was applied to the NACA 0015 wing. The results demonstrate a significant contribution of the boundary to the control effort.

We are investigating the rational approximation as an additive preconditioner for the nonzero base flow case. Since local dynamics is dominated by viscosity, this approximation should correctly describe the colocated sensing/actuation singularity in the optimal feedback kernel. As a first step, we are investigating a shear flow where the Fourier transform in the streamwise direction can be used to simplify the problem. We intend to compare the performance and quality of numerical results in the preconditioned formulation with those obtained directly. The insight gained in this study will provide guidance for the development of numerical schemes for the full NACA 0015 wing case at moderate Reynolds number flows.

### *The Coral Project*

The cost of developing complex computer components such as CPUs has become so high that scientific applications alone cannot carry the full burden. In the future, scientific computing will have to use mass market leverage to overcome the cost barrier. A cost-effective alternative to high-end supercomputing was pioneered by Beowulf, a cluster of commodity PCs. By now, high performance Beowulf clusters can be built using fast commodity PCs and switched Fast Ethernet. We want to explore the benefits and the limitations of this approach, based on applications of interest to ICASE.

Based on the available performance and price data, we created a list of configurations and at each price level selected the dominant configuration. After a discussion of various application benchmarking requirements, a system consisting of 32 Pentium II 400 MHz nodes and a dual CPU server was selected. The system's aggregate peak performance using multiple copies of the ATLAS benchmark exceeds 10 Gflop/s, while sustained performance on CFD applications is about 1.5 Gflop/s. Our benchmarks show perfect scaling with balanced coarse grained parallel codes. Fine grained codes show reasonably good scaling with the number of processors. During benchmarking, we discovered and resolved a performance limitation of the underlying TCP data transport protocol. Coral has an excellent price/performance ratio, almost an order of magnitude better than an equivalent supercomputer. This conclusion applies primarily to balanced coarse grained applications (e.g., domain decomposition codes).

We expect to refine Coral's performance through further benchmarking, and to use this system in solving some real problems. Since the cost of performance is rapidly decreasing, we hope to enhance and expand

this cluster in the future.

The Coral Project was initiated by Piyush Mehrotra and Tom Crockett. Additional benchmarking was done by David Keyes and Brian Allan.

## **DIMITRI J. MAVRIPLIS**

### *Large-scale Unstructured Mesh Computations Using a Parallel Multigrid Solver*

Unstructured mesh Navier-Stokes solvers offer great potential for reducing the turnaround time associated with complex geometry aerodynamic analysis. For accurate computation of complicated aerodynamic flows, very high resolution grids are required. Furthermore, the large computational overheads associated with unstructured mesh methods require the use of efficient solution algorithms which can be ported to massively parallel architectures. The purpose of this work is to demonstrate the feasibility of performing very large scale unstructured mesh computations in a production setting using existing parallel machines.

A low memory, rapidly converging unstructured multigrid algorithm has been developed and ported to parallel computer architectures. The fine and coarse levels of the unstructured multigrid algorithm are all partitioned sequentially before being distributed on the target parallel machines. Because the algorithm makes use of implicit line solves, the partitioning must be executed in such a way that the implicit lines of the various mesh levels are not intersected by processor boundaries. This is achieved by contracting the mesh graph along the implicit lines and partitioning the contracted (weighted) graph rather than the original graph of the mesh, which is then used to infer the final mesh partition upon de-contraction. The communication patterns (which remain static for the duration of the analysis) are then precomputed and stored. The implementation of the parallel solver is based on the MPI communication primitives.

Good scalability of the unstructured mesh multigrid solver has been demonstrated on medium size problems involving several million grid points on both a CRAY T3E-600, using up to 512 processors, and an SGI Origin 2000, using up to 128 processors. A complete high-lift aircraft geometry case has been solved on a grid of 25 million points in 4.5 hours on 512 processors of the Cray T3E. The same case has also been run on 1450 processors of a CRAY T3E-1200E, which required just over one hour of compute time.

The current solver has also been benchmarked on the ASCI Red and ASCI Blue-Pacific parallel computers, illustrating good scalability as well on these machines.

Future work is concentrated on enabling the solution of even larger cases, up to 100 million grid points. This will require the parallelization of all preprocessing operations such as mesh partitioning and coarse multigrid level construction. This effort is viewed as the first step towards developing a practical large eddy simulation capability for aircraft configurations.

## **CHI-WANG SHU**

### *High-order Discontinuous Galerkin Method and WENO Schemes*

Our motivation is to have high-order non-oscillatory methods for structured and unstructured mesh which are easy to implement for parallel machines. The objective is to develop and apply high-order discontinuous Galerkin finite element methods and weighted ENO (WENO) schemes for convection dominated problems. The applications will be problems in aeroacoustics and other time-dependent problems with complicated solution structure.

Jointly with Harold Atkins (NASA Langley), we are continuing in the investigation of developing the discontinuous Galerkin method to solve the convection-dominated convection diffusion equations. Emphasis

for this period is put upon studying the stability and accuracy issues involving both internal and domain boundary conditions. Discontinuous Galerkin method for 2D incompressible flow is also under development jointly with Jian-Guo Liu (University of Maryland). Jointly with Changqing Hu (Brown University), we have been pursuing adaptive methods using structured and unstructured high-order weighted ENO schemes. Preliminary results using a structured WENO code on the double Mach reflection problem indicate good resolution and a saving of 75% in terms of spatial mesh points over the uniform mesh code.

Research will be continued for high-order discontinuous Galerkin methods and weighted ENO methods and their applications.

## DAVID SIDILKOVER

### *Factorizable Schemes and Essentially Optimal Multigrid Solvers for the Flow Equations*

The main objective of this work is to develop discretization schemes that facilitate construction of the essentially optimal multigrid solvers for the equations of steady compressible flow. Our first target is the Euler equations in two dimensions. However, the methodology being developed is very general. It can be extended to Navier-Stokes equations and to three-dimensional problems.

A *factorizable* high-resolution scheme for the compressible Euler equations has been constructed. The *factorizability* property is crucial for constructing essentially optimal multigrid solvers, since it makes it possible to distinguish between the advection and full-potential factors of the system on the level of the discrete scheme. The key ingredient of such a solver is a relaxation procedure that relies on the auxiliary potential and stream-function variables and, therefore, utilizes the factorizability property. Another important implication of the factorizability property is that the scheme should not lose accuracy for the low Mach number flow. The proposed approach also allows the combination of *h*-ellipticity and high-resolution properties in one scheme.

The current work is devoted to extending the scheme/solver to general body-fitted grids. Extensions of the approach to viscous and three-dimensional problems are in progress as well.

## SEMYON TSYNKOV

### *Artificial Boundary Conditions for Aerodynamic and Aeroacoustic Computations*

Many typical problems in aerodynamics and aeroacoustics, including those that present immediate practical interest, e.g., flows around aircraft and problems of acoustic radiation/propagation/scattering, are formulated on infinite domains. It is, therefore, obvious that any numerical methodology for solving such problems has to be supplemented (or, rather, preceded) by some technique that would lead to a finite discretization. Typically, the original domain is truncated prior to the actual discretization and numerical solution. Subsequently, one can construct a finite discretization on the new bounded computational domain using one of the standard techniques: finite differences, finite elements, or other. However, both the continuous problem on the truncated domain and its discrete counterpart will be subdefinite unless supplemented by the appropriate closing procedure at the external computational boundary. This is done by using artificial boundary conditions (ABC's); the word "artificial" emphasizing here that these boundary conditions are necessitated by numerics and do not come from the original physical formulation.

At the current stage of the aforementioned project, we are focusing on the following two research topics. First, we construct highly accurate global boundary conditions for the calculation of steady-state flows using

the new generation of advanced factorizable finite-difference schemes and fast multigrid solvers. For the initial test cases the boundary conditions are obtained analytically via conformal mappings; at later stages we will employ the difference potentials method which has already demonstrated excellent performance in our previous work. The new schemes themselves have already led to a multifold reduction in the solution time (compared to the standard methods); when combined with the advanced external boundary conditions that allow for an order of magnitude decrease in the domain size without loss of accuracy, the new methodology may potentially result in more than two orders of magnitude overall reduction in the configuration analysis cycle. Second, we develop the exact ABC's for time-dependent problems. The approach is based on exploiting the weak lacunae in numerical solutions of the wave-type equations. This allows effective restriction of the temporal nonlocality of the ABC's, otherwise the procedure would be prohibitively expensive. We have studied the lacunae both analytically and experimentally and have already calculated the solutions to some model problems for the wave equation using the new ABC's methodology; the results seem very promising. A series of conference and journal papers is in preparation on both foregoing subjects.

Future research in the framework of this project will primarily concentrate on developing the unsteady ABC's algorithms for problems in acoustics, including the advective case, and electromagnetics.

This research was conducted in collaboration with V. Ryaben'kii, D. Sidilkover, S. Abarbanel, and J. Nordstrom (ICASE) and V. Vatsa, T. Roberts, C. Swanson, J. Thomas, and H. Atkins (NASA Langley). The project is supported by the Director's Discretionary Fund.

## PHYSICAL SCIENCES, FLUID MECHANICS

**RICHARD W. BARNWELL**

### *Hyperbolic Reynolds Stress Model for Turbulent Boundary Layers*

The boundary layer equations for incompressible mean flow with the turbulence model provided by the Reynolds stress equations are shown to be hyperbolic in the outer region where convection and diffusion dominate. Because diffusion is of inconsequential magnitude in the turbulent interior, it can be either ignored or approximated appropriately there so that the governing equations are hyperbolic across the entire turbulent part of the boundary layer. Consequently, hyperbolic solution techniques can be used to advantage to solve the turbulent boundary layer as Peter Bradshaw did over 30 years ago with a more approximate formulation. The hyperbolic solutions so obtained depend on conditions immediately upstream of the solution point and may give a better representation of the diverse behavior in complex three-dimensional boundary layers than traditional parabolic solutions.

Closure assumptions are required to relate the diffusion terms, which are dominated by derivatives of time-averaged triple products of the fluctuating velocity components, to the Reynolds stresses. The traditional approach is to replace the triple products with terms involving derivatives of the Reynolds stresses and solve the resulting parabolic problem. Experimental data show that the Reynolds stresses vary algebraically with distance from the mean boundary layer edge in the outer region where convection and diffusion dominate, and an asymptotic analysis shows that such functions satisfy a differential equation which renders the traditional differential representations of the triple products equivalent to the algebraic representation developed by Bradshaw. The result is a set of hyperbolic governing equations with fewer modeling constants than the corresponding parabolic set. In the hyperbolic approach the additional data are provided by initial conditions. The hyperbolic stress model is used to explain why the lateral spreading rate of a turbulent wedge in a laminar boundary layer is so much larger than the vertical boundary layer growth.

The next task is to compare the results of this method to those of other methods and experimental data.

**SANG-HYON CHU**

### *Development of Microwave-driven Smart Material Actuator*

“Wireless” control of actuators with microwave offer tremendous advantages over hard-wired actuators, especially for space applications such as the Next Generation Space Telescope (NGST), in which thousands of discrete actuators are required to affect high precision distributed shape-control of the primary reflector. This new concept alleviates the need for hard-wired connections resulting in significantly simpler system designs and lower system mass.

3x3 rectenna patches built at JPL were tested in an anechoic chamber by modulating microwave power level, frequency, incidence angle, and polarization angle. The PZT 5A multilayer piezoelectric actuator was selected as the smart actuator and tested under a direct coupling with a 3x3 rectenna. The obtained experimental results indicate that the multilayer piezoelectric actuator can be successfully utilized with a wide degree of controllability when the 3x3 patch rectenna converts microwave energy to DC power that, in turn, drives the actuator.

The nature of dispersion of microwave might cause energy loss during transmission. The concept of power allocation and distribution will be considered for this reason. Logic circuits embedded in rectennas

will control power collection and allocation to feed DC power to any actuator where optical correction is necessary. A prototype of a power distribution circuit will be fabricated and improved to meet all required characteristics in the future.

## **AYODEJI DEMUREN**

### *Streamwise Vorticity Generation in Jets*

Experiments have shown that three-dimensional jets can be used to enhance mixing and entrainment rates in comparison to axisymmetric jets. A fundamental understanding of the dynamics of complex, turbulent jets is required for their prediction and control. Understanding of the evolution of the streamwise vorticity fields is essential. Experiments have used streamwise and azimuthal vorticity dynamics to explain the presence or absence of axis-switching in experimental measurements of 3:1 aspect ratio rectangular jets with different initial conditions. This study showed that the presence of streamwise vorticity pairs with out-flow rotation (pumping fluid from the core to the ambient perpendicular to the major axis plane) produced axis switching while pairs with the opposite sense of rotation did not. However, in jets with no streamwise vorticity at discharge, some other mechanism must originate it.

Generation mechanisms are investigated via Reynolds-averaged (RANS), large-eddy (LES) and direct numerical (DNS) simulations of laminar and turbulent rectangular jets. Complex vortex interactions are found in DNS of laminar jets, but axis-switching is observed only when a single instability mode is present in the incoming mixing layer. With several modes present, the structure is not coherent and no axis-switching occurs. RANS computations also produce no axis-switching. On the other hand, LES of high Reynolds number turbulent jets produce axis-switching even for cases with several instability modes in the mixing layer. Analysis of the source terms of the mean streamwise vorticity equation through post-processing of the instantaneous results shows that a complex interaction of gradients of the normal and shear Reynolds stresses is responsible for the generation of streamwise vorticity which leads to axis-switching. RANS computations confirm these results.  $K - \epsilon$  turbulence model computations fail to reproduce the phenomenon, whereas algebraic Reynolds stress model (ASM) model computations in which the secondary normal and shear stresses are computed explicitly succeeded in reproducing the phenomenon accurately.

More quantitative comparisons to experimental data are planned.

## **SHARATH S. GIRIMAJI**

### *Pressure-strain Correlation Modeling: Testing and Validation*

At the second moment closure level, accurate modeling of turbulent flows is contingent upon accurate modeling of the pressure-strain correlation term. Development of pressure-strain correlation models valid for complex flows is the objective of this project.

We have entered the final stages of validating and fine-tuning of the model. After successful validation in a variety of benchmark problems, more subtle issues on the manner of interpolation between extreme states are being addressed. While matched asymptotic expansion techniques are theoretically sound, they appear to lead to very complex model forms. Other avenues are being explored.

Further testing and systematic development for intermediate states of turbulence will come next.

### *Rotating Turbulent Flows*

The effect of rotation on turbulence still remains an enigma in many practical flow situations. Our objective is to understand the behavior of irrotational fluctuations in a flow with strong mean-flow rotation.

While the effect of rapid rotation on rotational fluctuations is well described by the Taylor-Proudman theorem, the behavior of irrotational fluctuations is not well known. We demonstrate that the Navier-Stokes equations permit a large family of irrotational solutions in two-dimensional or rapid rotation limits. This could lead to improved insight into the behavior of turbulence in rotating flows.

The importance of irrotational fluctuations in turbulence needs to be further expounded.

This research was conducted in collaboration with J.R. Ristorcelli (Los Alamos National Laboratory).

### *Non-equilibrium Algebraic Reynolds Stress Modeling*

Computationally viable, yet physically accurate turbulence models are needed for large-scale, practical flow computations. We develop such a model starting from the physically sophisticated but computationally expensive second-order closure.

The theory of complex dynamical systems is being studied to develop new reduction procedures. A scheme based on minimization of evolution potential was developed and is currently undergoing close scrutiny. This appears to offer important advantages over previous methods. A simple procedure for identifying the slow (master) variables is developed.

Extensive testing of the slow variable selection criterion and the reduction procedure would come next.

## **C.E. GROSCH**

### *Simulation of Supersonic Jet Mixing by Tabs in Lobe Ejectors*

Mixing enhancement of high- and low-speed streams is utilized as a means to improve efficiency of supersonic combustors, reduce aircraft signatures, and control high-speed jet noise. One common method of mixing enhancement is to use lobe mixer ejectors. Another is to place tabs on the edges of the jets. In the main, experimental studies are available to evaluate the performance and guide the design of these mixers. The objective of this research is to use numerical simulation to examine the performance of lobe ejectors, both with and without tabs, in order to understand the physics of the mixing and how it is affected by changes in the parameters of these devices.

A set of numerical calculations are carried out using the compressible, three-dimensional, time-dependent Navier-Stokes equations. Tabs are modeled by pairs of counter rotating vortices. Various geometric configurations of the lobe mixers are simulated with periodic side boundary conditions to simulate an array of these devices.

The simulations of the lobe mixer without tabs show that the jet becomes unstable and oscillates in the "garden hose" mode. For a particular lobe geometry and velocity ratio, the oscillation has a constant, narrow band, frequency near the inflow. Further downstream the amplitude grows and the motion becomes nonlinear leading to spectral broadening. Typical Strouhal numbers of the narrow band oscillation is about 0.45. The physics of this phenomena is related generation of streamwise vorticity at the edges of the jet. As the disturbances become nonlinear, rapid mixing between the supersonic and subsonic jets occurs and, by about halfway down the channel, the jet and coflow become nearly fully mixed. A set of simulations of the same geometry with tabs has begun. The results of the first of these has been partially analyzed.

Future experimental and numerical studies are required to more clearly define the initial induced vorticity field in the round jet. It is hoped that future experiments will use PIV imaging to measure the cross-stream vectors. The experimental data could then be used to set the inflow conditions for the simulations.

Further calculations are planned for the lobe mixer including varying the geometry and varying the placement of the tabs on the sides of the lobes.

## **ROGER HART**

### *Flow Diagnostics Using Laser-induced Thermal Acoustics*

The non-intrusive optical measurement of gas-phase parameters such as temperature, flow velocity, and pressure is of considerable utility in understanding the airflow around a test body in a wind tunnel. Laser-induced thermal acoustics (LITA) is a relatively new optical diagnostic method that has great promise for becoming a practical, accurate flow characterization tool. Two laser pulses are employed in LITA. The first pulse creates a pair of counterpropagating acoustic wavepackets. The second pulse is diffracted by the wavepackets onto a detector. Analysis of the various features of the LITA waveform allows the determination of the speed of sound in the medium (and thus the bulk temperature), one or more components of the flow velocity, and the density or pressure. Advantages of LITA as compared to other, better-developed diagnostics are: LITA allows seedless velocimetry; LITA measurements take only about one microsecond, giving the potential for very high repetition rates for the study of turbulent flows; and LITA gives excellent ( $\sim 1\%$ ) single-shot accuracy and precision. The goal of the current work is to completely understand the physics of the LITA measurement process and to embody that understanding in a quantitative model which has been carefully validated against laboratory experiments.

The fundamental optical and acoustical mechanisms of LITA are well understood; nevertheless, combining these to create a model that can accurately and robustly duplicate the results of well-controlled experiments has involved considerable effort. On the experimental side, we currently make measurements in calibrated air flows using standard laboratory style lasers and optics, as this allows the greatest flexibility and control, though thought is being given to simplifying and hardening the equipment for use in production wind tunnels. Modeling currently combines fairly simple models for low-amplitude (linear regime) sound waves and standard optical diffraction theory. One recent accomplishment was learning how to correctly include the effect of the finite size of the acoustic wavepackets on the decay rate of the LITA waveform. The decay of the signal limits the precision of measurements of temperature and velocity, and the rate of the decay is a critical piece of information for determining pressure, so this is of some importance for the application of LITA.

The major unresolved modeling issue involves explaining certain systematic differences observed among the decay rates of the three spectral components that make up the LITA signal. An additional series of experiments is being considered to help constrain our modeling efforts. This research was conducted in collaboration with R.J. Balla and G.C. Herring (NASA Langley).

## **LI-SHI LUO**

### *Lattice Boltzmann Scheme for Flow-structure Interaction*

One important problem in the applications of the lattice Boltzmann equation to various flow problems is the interaction between fluid flow and solid boundaries, i.e., the implementation of boundary conditions



in fluid-structure interfaces. The moving boundary problem in high Reynolds flow poses a challenge to traditional CFD methods. Usually, turbulence modeling has to be employed in such cases. The present work uses the method of the lattice Boltzmann equation (LBE) to simulate the flow-structure interaction problem.

With the LBE method, boundary conditions for objects with complicated geometries are easy to implement. We intend to implement a computationally efficient boundary condition for moving boundaries in flows with high Reynolds number. Various schemes combining existing bounce-back type boundary conditions with interpolation (or extrapolation) are under theoretical study and numerical test.

A paper entitled “An Accurate Curved Boundary Treatment in the Lattice Boltzmann Method,” authored by Renwei Mei, Li-Shi Luo (ICASE), and Wei Shyy has been submitted to the Journal of Computational Physics. Currently we are working on boundary conditions for a moving boundary.

The present work has been funded by NASA Langley Research Center under the program of “Innovative Algorithms for Aerospace Engineering Analysis and Optimization.” The Co-PI’s of the proposal for the present work are Renwei Mei (UFL), Li-Shi Luo, and Wei Shyy (UFL). The collaboration also includes Pierre Lallemand (Director, ASCI-CNRS, Univ. Paris-Sud), and Dominique d’Humières (ENS, Paris).

#### *Lattice Boltzmann Model for Non-ideal Gases*

The key issues in the study of multi-phase (e.g., liquid-vapor) flows are the modeling of interfaces and phase transition among different phases. It is difficult to use the Navier-Stokes equations to model the inhomogeneous multi-phase flows because the interfacial tracking is a laborious computation. In the past few years, a number of lattice Boltzmann models have been developed to model multi-phase flows. However, the multi-phase lattice Boltzmann equation is still lacking a rigorous theoretical basis. For instance, previous multi-phase lattice Boltzmann models do *not* have a consistent equilibrium thermodynamics. The present work applies the *Enskog theory* of hard spheres to revise the theory of the multi-phase lattice Boltzmann equation.

With the Enskog theory we were able to derive a new multi-phase lattice Boltzmann model which has a consistent equilibrium thermodynamics. We have *rigorously* demonstrated the deficiencies in the previous multi-phase lattice Boltzmann models and provided a systematic procedure to derive a *correct* multi-phase lattice Boltzmann model based upon the Enskog theory (or the revised Enskog theory). A brief account of the present work has been published in Physical Review Letters and as an ICASE report. An extended version of the work has been submitted to Physical Review E and a corresponding ICASE report is in preparation.

We intend to derive a thermodynamically *consistent* multi-component lattice Boltzmann model in the future based upon the same methodology.

### **ALEX POVITSKY**

#### *Computation of Three-dimensional Acoustic Fields*

Our goal is to improve parallelization efficiency of sets of linear banded systems which represent a core part of implicit and compact solvers. To use processors for other tasks while they are idle from recursive algebraic computations, we run processors by a schedule rather than by communication. This schedule is generated before CFD computations are executed.

To improve parallelization efficiency, we combined our Immediate Backward Pipelined Gaussian Elimination (IB-PTA) with the known Two-Way Pipelined Gaussian Elimination (TW-PTA) to obtain the Immediate Backward Two-Way Pipelined Thomas Algorithm (IBTW-PTA). To generate the processor schedule, we use recursive algorithm for the row of first  $P/2$  processors as described in our ICASE Report and make symmetric reflection of this schedule for the last  $P/2$  processors. Then we include exchange of the forward-step coefficients between the  $(P/2)^{th}$  and  $(P/2 + 1)^{th}$  processors and solution of  $2 \times 2$  system. These tasks are performed immediately after completing the forward-step computations for each group of lines on middle processors. Measurements on CRAY-T3E show an advantage of the proposed algorithm over the standard PTA, the TW-PTA and the IB-PTA for 8 and 16 processors-in-row. Reduction of processor idle time and large optimal size of the pocket of lines (low communication latency time) ensure low parallelization penalty of the proposed algorithm.

We are working on implementation of this algorithm to a 3D aeroacoustic solver (with P. Morris); implementation of processor schedule for multigrid line solvers (with B. Diskin); for the front-type solvers where grid lines are data-dependent; and for the multi-zone solvers where a processor might handle pieces of different grids.

### C.-C. ROSSOW

#### *Investigation of the Properties of the MAPS Flux Splitting Scheme*

Several efforts have been focused on the development of discretization methods that combine the accuracy of flux-difference splittings in capturing of shear layers with the robustness of flux vector splittings in capturing strong shock waves. One recent contribution to this class of hybrid flux splittings is the MAPS (Mach number based Advection Pressure Splitting) scheme. Significant features of the MAPS scheme are its simplicity, its robustness, and the fact that no entropy condition is required. Further research revealed that the scheme is very similar to the Roe flux-difference splitting, with the exception that no intermediate state needs to be computed. It was found that in the original MAPS formulation only the compressible terms of the Roe-scheme are retained. Including the incompressible terms of the Roe-scheme into the MAPS formulation extended MAPS to incompressible flows. In the research to be conducted, the connection of the MAPS discretization with the Roe-scheme shall be further exploited. On the one hand, a better understanding of the terms necessary for low Mach number preconditioning is sought. On the other hand, research will be directed towards convergence acceleration by implicit methods. For implicit schemes, the flux Jacobians need to be evaluated, which is well established for the Roe-scheme. Due to the similarity of MAPS and Roe discretization, it is expected that simplifications to the implicit operators can be made. This may be essential for unstructured methods where the directional techniques from structured codes for implicit residual smoothing cannot be applied straightforwardly, but in 3D fully-implicit methods are still prohibitive due to storage requirements.

The first area of research is the formulation of a consistent preconditioning matrix. An analysis of the Roe-scheme revealed that in the incompressible limit pressure terms dominate the artificial dissipation. These pressure terms are scaled by the inverse of the speed of sound. In order to remove the stiffness at incompressible flows, the speed of sound in these terms is artificially reduced, thus making these terms even more dominant. It appeared logical that these artificially increased pressure differences have to be balanced by properly scaled, artificially introduced time-derivatives of pressure. Adding these pressure time-derivatives to the equations written in strong conservation form leads to a preconditioning matrix being identical to the Choi/Merkle preconditioning in the incompressible limit. However, due to the proper

scaling, for compressible flows the nonpreconditioned compressible equations are recovered, a feature not shared by the original Choi/Merkle preconditioner.

In the second area of research, the possibility of exploiting the MAPS formulation for an acceleration technique similar to implicit residual smoothing will be investigated. In the MAPS formulation, advective and pressure terms appear separately. Using an implicit, scalar smoothing for the advective terms in each equation while treating the pressure terms explicitly as a source term may result in an acceleration technique similar to the directional smoothing well established in structured methods. However, the directional dependence will be avoided, making the technique feasible for unstructured methods. Depending on the results obtained with this simplified implicit scheme, it may be intended to incorporate the MAPS discretization into a fully implicit formulation.

## ROBERT RUBINSTEIN

### *Shock Wave Propagation in Weakly Ionized Gases*

It has been proposed that the mechanism responsible for anomalous properties of shock waves in weakly ionized gases could be identified by measuring the relaxation time of these properties following extinction of the plasma source, and matching it to the relaxation times of the nonequilibrium phenomena known to exist in weakly ionized gases. When these relaxation times cannot be measured directly, they are inferred theoretically, usually by assuming relaxation from a state nearly in thermal equilibrium. This proposal therefore requires the understanding of relaxation from a steady state far from thermal equilibrium. In order that the matching be unambiguous, the relaxation rates in the weakly ionized gas must be known precisely.

We investigated this relaxation for two typical problems: the relaxation of a steady state described by a power-law distribution function, and the relaxation of a non-equilibrium steady state in a gas of light particles diffusing in a gas of heavy particles. In both examples, it is found that relaxation is much slower than relaxation from a near-equilibrium state. The explanation is that if the Boltzmann equation is satisfied away from the momentum space sources and sinks which maintain the non-equilibrium steady state, relaxation to thermal equilibrium requires that the effects of extinguishing the sources and sinks diffuse over all of momentum space. This relaxation can be very slow. We conclude that the relaxation times in a non-equilibrium weakly ionized gas may be evaluated incorrectly if exponential relaxation from a near-equilibrium state is assumed. A correct calculation will require a more detailed molecular model of the weakly ionized gas, at the level of a Boltzmann equation at least.

The pressure fields produced in the regions of unbalanced charge ahead and behind the shock have been proposed as sources of increased sound speed and anomalous shock properties. The possibility of non-ideal gas corrections to the equation of state due to large electrostatic forces will be investigated next.

This research was conducted in collaboration with A.H. Auslender (NASA Langley).

### *Boundary Layer Receptivity in the Presence of Random Surface Roughness and Acoustic Excitation*

There is still no well-established procedure for incorporating transition in turbulence calculations. While aerodynamic flows can be computed successfully using any of several different turbulence models if the transition location is prescribed in advance, no single turbulence model can reliably predict transition. If transition is computed incorrectly, the entire flow calculation is generally unsatisfactory.

As part of a larger program of integrating transition and turbulence models, the first stage of transition, boundary layer receptivity, is being considered from a probabilistic viewpoint. The analysis allows both

the surface roughness distribution and the acoustic excitation, which combine to excite Tollmien-Schlichting waves, to vary randomly. A simple stochastic differential equation is being investigated as a model of this process. Preliminary Monte Carlo simulations demonstrate the effect of random surface roughness in enhancing receptivity.

The analysis will be extended to permit prediction of the probability density function of receptivity amplitude as a function of downstream position. The calculation will also be extended to more realistic models of receptivity, including downstream variability of the growth rate of Tollmien-Schlichting waves.

This research was conducted in collaboration with S.S. Girimaji (ICASE) and C.L. Streett (NASA Langley).

#### *Theory of Rotating and Stratified Turbulence*

The theory of weak turbulence describes the inertial range structure of rotating turbulence, considered as a system of interacting inertial waves. It is natural to ask whether a similar description of the dissipation range is possible when wave effects persist into the dissipation range. This analysis is also motivated by the known anisotropy of energy transfer in rotating turbulence: unlike non-rotating turbulence, in which energy is transferred from larger to smaller scales of motion, in rotating turbulence, energy is simultaneously transferred to the plane perpendicular to the rotation axis.

It is known that dissipation range interactions are between modes with nearly collinear wavevectors. It is shown that the dispersion relation of inertial waves permits such interactions to be resonant only when the wavevectors are nearly perpendicular to the rotation axis. Accordingly, the dissipation range in strongly rotating turbulence is concentrated near this wavevector plane. Since inertial range interactions transfer energy into this region, it is plausible that the dissipation range should be concentrated near it.

This research was conducted in collaboration with Ye Zhou (ICASE and Tuskegee University).

#### **NAIL YAMALEEV**

##### *A High-order Accurate Method on a Moving Grid Adapted to the Solution*

It is known that the attainment of high-order accuracy for problems with shocks is problematic, since a first-order error introduced by the shock-capturing procedure can persist globally downstream. One of the most effective ways to reduce this error is to diminish the grid spacing in the shock region alone rather than refine the grid in the entire computational domain. The main purpose of the present work is to elaborate a high-order accurate shock-capturing scheme on a moving grid dynamically adapted to the solution, that enables one to increase the resolution of high gradients as well as improve the accuracy of the solution in smooth flow regions.

High-order linear and nonlinear shock-capturing schemes are used to solve the 2D unsteady Euler equations written in general curvilinear coordinates. For the linear shock-capturing scheme, the interpolation set for the approximation of the solution is fixed as a function of grid location. For the nonlinear scheme, the solution is represented by using a high-order accurate polynomial reconstruction, so that the adaptive stencils employed in the high-order spatial operator are biased towards the smoothest information available. To generate a grid including such important properties as smoothness, orthogonality and adaptation simultaneously, the variational approach proposed by Brackbill and Saltzman is employed. Since the Jacobian of transformation depends on the temporal coordinate, the geometric conservation law originally introduced by Thomas and Lombard must be satisfied. Then the geometric conservation law equation is solved numerically

along with the flow conservation law using the same conservative difference operators as those employed for approximating the governing equations. The high-order accurate flow solver and the adaptive grid generator have been implemented. We are currently joining these codes so that the geometric conservation law is satisfied automatically at each time step.

We plan to apply the present method to calculate both steady and essentially unsteady flows with shocks.

This research was conducted in collaboration with M. Carpenter and J. Thomas (NASA Langley).

**YE ZHOU**

*On Higher-order Dynamics in Lattice-based Models Using Chapman-Enskog Method*

Compared to traditional methods in computational fluid dynamics (CFD), the lattice-based models are simple and easy to implement on computers. The advantages and disadvantages of the original lattice gas automata (LGA) have been well documented. The lattice Boltzmann equations (LBE) were later introduced to remove some of the drawbacks. A further simplification to the LBE is achieved using the BGK procedure (LBGK). Indeed, it is well established that the Navier-Stokes equation can be deduced at low-order expansion of Chapman-Enskog expansion. Many authors further asserted that the Burnett-like equation could be obtained by performing higher-order using Chapman-Enskog expansion. The motivation of this work is to carry out these higher-order Chapman-Enskog expansions to investigate whether it is consistent to do so.

We found that two conditions determine whether the lattice-based models could or could not have higher-order dynamics when classical Chapman-Enskog expansion is used. These conditions are a number of conservation laws and the space and time discretization. The pure diffusion model, a system with only one conserved quantity, is first presented to illustrate that the higher-order dynamics is allowed. We then turned our attention to the lattice-based hydrodynamics equations. After noting the feature of non-commutative cross time derivative, we demonstrate how Burnett-like equations could be obtained for lattice-based hydrodynamics models using the classic Chapman-Enskog expansion method.

The results reported in this work can be used to analyze theoretically systems where hydrodynamic description may break down, a typical example is simulations of the micro-electronic mechanical systems (MEMS).

This research was conducted in collaboration with Y.H. Qian (Columbia University).

## COMPUTER SCIENCE

**PO-SHU CHEN**

### *Parallel Solution of Coupled Aeroelastic Problems*

The accurate prediction of aeroelastic response is essential in the design of high performance aircraft. It requires solving the coupled fluid and structure equations simultaneously. The objectives of this research are to investigate a variety of different approaches for solving aeroelastic problems, to establish a proper module between structure and fluid simulations, to solve the aeroelastic response, and to research a better integration algorithm for communication between fluid and structure equations.

A new package, Load and Motion Transfer (LMT), has been developed to be a 'bridge' between CFD and FEM software for aeroelastic simulation. It is capable of interpolating the initial nodal coordinates of the fluid mesh from the structure nodal displacement, and to integrate the structure nodal force from the fluid pressure. It is superior to the FASIT code, currently being used by the MDO branch of NASA Langley, in terms of flexibility, accuracy, and user-friendliness.

Since the reliable transfer program is available, the next stage is a simple static aeroelastic problem. The fluid research code developed by Dimitri Mavriplis and structure research code developed by Charbel Farhat have been selected for this purpose. However, the package here is capable of solving the steady state of the aeroelastic problems only. It cannot solve real time-dependent problems, like vibration. The second stage of improvements is to consider the proper approach for the heavy communication aeroelastic package. The details of the approach are still in discussion.

This research was conducted in collaboration with Tom Zang and Anthony Giunta (NASA Langley), Dimitri Mavriplis (ICASE), and Charbel Farhat (University of Colorado).

**THOMAS W. CROCKETT**

### *Porting PGL to Beowulf-class PC Clusters*

The development of low-cost computational clusters based on commodity processors and networking components has become an important new trend in parallel computing. Many organizations have installed such systems, and many more are planning to do so. In the near future, Beowulf-class clusters could become the platform of choice for many challenging scientific and engineering computations. To derive maximum benefit from these systems, users will need the same tools and capabilities that have been developed for use on proprietary parallel computing systems.

One of these tools is the PGL rendering system, developed at ICASE to provide runtime visualization support for parallel applications. PGL currently runs on half a dozen different MPP systems. We have recently been working to develop a version for Linux-based PC clusters, using ICASE's Coral system, a Beowulf-class cluster, as a development platform. Although we expected this to be straightforward, a number of problems have arisen involving compilers and low-level communication layers. Consequently, a substantial portion of our effort has involved installing and testing compilers, message passing libraries, network interfaces, and job schedulers. Serial and parallel versions of PGL are now running on the Coral cluster, using 400 MHz Pentium II processors and Fast Ethernet communication hardware. Serial performance on a benchmark suite is good, ranging from 70-107% of a 300 MHz Sun UltraSPARC II and 39-71% of a 250

MHz MIPS R10000. Parallel performance results are awaiting resolution of problems with Coral's network interfaces.

When testing and performance evaluation of the Linux/PC version of PGL is completed on Coral, we plan to release it to NASA's HPCCP/CAS community as part of PGL 1.2. Longer term plans include additional testing and algorithmic modifications for distributed shared memory architectures such as the SGI Origin2000 and HP Exemplar, where scalability has so far been poor. We also have plans to incorporate additional functionality in PGL, and to develop improved user interfaces for interactive applications.

### *Application of Parallel and Distributed Computing to Visualization and Data Assimilation Problems in the Atmospheric Sciences*

To implement the Vice President's vision of a Digital Earth, vast quantities of data from disparate sources must be integrated into an intuitive, accessible representation. NASA's Earth Science Enterprise sees Digital Earth as a promising framework for making much of its remote sensing data available to the scientific community and the general public. To implement the Digital Earth concept, many technologies will need to be brought to bear, among them visualization, networking, and high-performance computing.

We are exploring the potential for parallel and distributed computing and visualization techniques to contribute to the data processing and data assimilation requirements of Digital Earth. We have used ICASE's PGL rendering system to develop a prototype visualization application which combines a medium-resolution (9 km) elevation model of the Earth with a true-color surface map, including support for several different map projections. Preliminary performance tests have been conducted on Langley's 16-processor Origin2000 system, and on a network of Sun UltraSPARC workstations at ICASE. Although rendering performance is good, the results suggest that multi-resolution data representations and additional graphics functionality (such as triangle strips and more aggressive clipping algorithms), in addition to higher processor counts, are needed to deliver interactive performance with models of this size (18.7 million triangles). User interfaces which are tailored to the application will also be required, and we have begun evaluating Java for this purpose. In related activities, we served on Langley's Digital Earth Planning Team, and continued participating in meetings of the federal Inter-agency Digital Earth Working Group.

We plan to combine atmospheric data from Langley's LITE experiment with the digital terrain model described above to produce an interactive tool for visualizing vertical structure in the atmosphere. The ultimate goal is to develop a responsive, user-friendly system which will combine atmospheric data from a variety of sources to obtain a better understanding of the physical processes involved. We also want to investigate approaches for incorporating much larger terrain models, such as USGS's 30-arc-second global elevation dataset (933 million grid points). We hope that the techniques developed will lead us toward Digital Earth's goal of providing interactive access to multi-petabyte datasets, a challenge which is beyond the capability of current computing technology.

### **DAVID E. KEYES**

#### *Parallel Implicit Solvers for Simulation of Multiscale Phenomena*

The development and application of parallel implicit solvers for multiscale phenomena governed by PDEs are our chief objectives. Newton-Krylov-Schwarz (NKS) methods have proven to be broadly applicable, architecturally versatile, and tunable for high performance on today's high-end commercial parallel platforms (e.g., Cray T3E, SGI Origin, IBM SP). Both structured-grid and unstructured-grid CFD legacy codes have

been ported to such platforms and reasonable objectives for algorithmic convergence rate, parallel efficiency, and raw floating point performance have been met. However, architectural challenges have increased on the next generation of high-end machines, as represented, for instance, by the ASCI “blue” machines at Lawrence Livermore and Los Alamos National Laboratories, and also on Beowulf clusters, such as ICASE’s Coral. Our primary efforts are concentrated on algorithmic adaptations of NKS methodology appropriate for the emerging architectures and on evaluation of new software tools and methodology to get the most performance out of them.

The general approach embodied in the NKS family of algorithms is documented in previous ICASE technical reports, among other places. Specific emphases in the most recent reporting period include enhanced per-node floating point performance, multilevel preconditioning, optimization, and evaluation of NKS applications on the ICASE Beowulf system.

Per-node floating point performance has been a source of major consternation for users (and apologists) of high-end machines. Anecdotal evidence, such as a list of recent “Bell Prize” peak performance winners, indicates that sparse, grid-based computations do not stack up very competitively against other scientific simulations. We have shown that attention to cache line reuse in the organization and ordering of grid-based data that is iteratively dragged up and down the memory system in a typical PDE code can make an order of magnitude difference in execution time, apart from parallelism, and an experimental program to study this effect via hardware event counters is on-going. Our ultimate aims are to apply formal optimization techniques to the layout of program data for optimal register and cache residency, to prepare for “Processors-in-Memory” (PIM) programming that vendors have announced in future products, and to evaluate the algorithmic utility of *multivector* forms of sparse algorithms with better cached matrix reuse.

Single-level Schwarz preconditioning is sufficient for many purposes, especially unsteady or pseudo-time continuation applications. However, we have recently demonstrated on some highly nonlinear radiation transport applications that 2-level Schwarz methods, with a coarse level that is removed from the fine grid by many powers of two in density, is not only superior in convergence but can be somewhat superior in overall execution time, in spite of the global coordination required.

Optimization is usually the real goal of computational simulation capability. As a goal unto itself, parallel optimization is much studied, but optimization subject to a high-dimensional set of equality constraints coming from a discretized PDE is a situation in which the tail wags the dog. Following the leads of O. Ghattas and D.P. Young in this area, we are exploring the utility of the NKS “rootfinder” as a Lagrange-NKS optimizer.

In terms of peak performance, the ICASE Beowulf cluster is cost-effective hardware, but the software environment is co-critical. In tests of the same Euler benchmark used on the ASCI machines, we have shown (see the Coral webpages) that the Portland Group compilers are particularly effective on native non-cache-optimized code, with uniprocessor running times that beat the ASCI processors and also the same 400 MHz Pentium II with NT compilers. For cache-optimized code, the R10000 and Power2 are still somewhat superior, but the per-node performance of Coral is almost competitive, independent of economic considerations.

We will continue to develop NKS methods in implicit parallel CFD, examining a variety of algorithmic, programming paradigm, and architectural issues. We will also increase the complexity of the models in our NKS radiation transport work, in accordance with the ASCI project roadmap.

This research was conducted in collaboration with W. Kyle Anderson (NASA Langley), Dana Knoll (Los Alamos National Laboratory), Dinesh Kaushik, Nilan Karunaratne, and Xin He (Old Dominion University),



and Satish Balay, William D. Gropp, Lois C. McInnes, and Barry F. Smith (Argonne National Laboratory).

## GERALD LÜTTGEN

### *Statecharts via Process Algebra*

Statecharts is a visual language for specifying synchronous reactive systems which is popular among software engineers, despite the complexity of its step semantics. It extends finite-state machines by concepts of concurrency, hierarchy, and priority. Most Statecharts variants do not have a compositional semantics and, thereby, prohibit the reuse of specifications of systems' components. The reason for this prohibition is the subtle interplay between micro and macro steps, as imposed by Statecharts' synchrony hypothesis and the principle of causality. The focus of this research is to develop a compositional process-algebraic framework which is expressive enough to embed several Statecharts variants.

The process algebra that has been developed is inspired by timed process languages and unifies the principles of Statecharts semantics, such as concurrency, causality, and synchrony. It represents macro steps as sequences of micro steps which are enclosed by clock ticks. The benefits of this approach include the establishment of a compositional framework (1) which is suitable for embedding several Statecharts variants, (2) which is intuitive and simple since causal orderings are not encoded in transition labels, (3) which can be equipped with behavioral equivalences carried over from traditional process algebras, and (4) which allows for interfacing Statecharts to verification tools.

In the future, we hope to apply the insights between clock semantics and Statecharts semantics obtained during this research to develop a Statecharts variant which is suitable for specifying distributed reactive systems.

This research was conducted in collaboration with Rance Cleaveland (SUNY at Stony Brook) and Michael von der Beeck (TU Munich).

### *Applying Model Checking Tools to the Verification of Flight Guidance Systems*

Mode confusion is one of the most serious problems in aviation safety. Today's digital flight decks are too complex in order for pilots to be aware of the actual states – or modes – of all systems. A year ago, NASA Langley started an initiative to analyze the mode logic of a flight-guidance system to uncover weaknesses in its design which may lead to mode confusion. For this purpose, the mode logic was modeled as a finite state machine, and the theorem prover PVS was used to reason about the system. The objective of this research is to investigate whether model checking techniques – i.e., sophisticated, automated state-exploration methods – are able to achieve this task “better” than theorem proving.

In this light, the mode logic is modeled and analyzed by using three popular model-checking tools: Mur $\phi$ , SMV, and Spin. In general, all three tools are able to handle the task fairly well and promise to scale up. The modeling is most elegant in Mur $\phi$  and SMV since their specification languages match the characteristics of the mode logic as a modular, synchronous system. Mur $\phi$ 's rich language even allows for carrying over the PVS specification of the mode logic one-to-one, and its ability to specify and verify invariants enables the efficient verification of many properties related to mode confusion. For the latter, however, the temporal logic CTL – as employed in SMV – is more practical due to its flexibility to reason about system paths rather than system states. Moreover, SMV's model checker, which is based on Binary Decision Diagrams, is faster than the other tools and outperforms PVS by returning verification results instantly. Finally, diagnostic information generated by each of the three tools is as adequate as the information obtained when using PVS.

In the future, we will model larger parts of the digital flight deck, such that the model-checking techniques may investigate more complex problems related to mode confusion.

This research was conducted in collaboration with Victor Carreño (NASA Langley).

## KWAN-LIU MA

### *Image Graphs - A Novel Approach to Visual Data Exploration*

Effort spent generating and collecting data is wasted unless there are effective means to organize and understand this data. This fact poses a problem in some modern visualization research. For example, in volume rendering the current data handling and visualization technology cannot handle the sheer size of emerging datasets. While various efforts have been made to condense datasets and accelerate rendering calculations, little work has been done to coherently represent the process and results of this type of visualization. However, this information about the data exploration is knowledge that should be shared and reused. The objective of this research is to develop a mechanism which not only offers a representation of this knowledge but also serves as an interface for visual data exploration.

We use a graph-based approach to represent not only the results but also the process of data visualization. Each node in the graph consists of an image and the corresponding visualization parameters used to produce it. Each edge in the graph shows the change in rendering parameters between the two nodes it connects. We, thus, call this design *image graphs*. Image graphs are not just static representations since users can interact with a graph to review a previous visualization session or to perform new rendering. In particular, operations which cause changes in rendering parameters can propagate through the graph. Image graphs help streamline the process of visual data exploration in two ways. First, the graphs give the user a representation of the relationship between the visualization parameter changes and the images produced using them. Often these relationships are not obvious just through inspection of the rendered images. An understanding of how specific rendering parameter changes will affect the image output is important because it reduces the number of images the user must produce to find parameters which yield a useful image, and these images can be quite time consuming to produce. Second, the dynamic features of the graphs, such as annotation and automatic pruning, facilitate collaboration and animation. They also help speed the search for good rendering parameters by allowing users to perform operations on groups of nodes. These operations include simple modification of rendering parameters, combination of nodes to form “child” nodes with their properties, and propagation of modifications through the graph. We have implemented a web-based volume visualization system which uses the image graph design for the purpose of supporting remote and collaborative visualization.

We are presently designing a comprehensive user study to understand the extent to which the image graphs can be shared and reused, and to refine the design of the visualization system we have built and its image graph interface. Furthermore, we think image graphs would be useful for any type of data exploration problem which produces images of data as a function of some set of parameters. Therefore, in addition to volume visualization, other possible applications include radiosity calculations, 2D image filtering, and polygon-based rendering. Our future work includes demonstrating that our approach is indeed useful for these other problem domains.

## PIYUSH MEHROTRA

### *Arcade: A Distributed Computing Environment for ICASE*

Distributed heterogeneous computing is being increasingly applied to a variety of large-size computational problems. Such computations, for example, the multidisciplinary design optimization of an aircraft, generally consists of multiple heterogeneous modules interacting with each other to solve the problem at hand. Such applications are generally developed by a team in which each discipline is the responsibility of experts in the field. The objective of this project is to develop a GUI-based environment which supports the multi-user design of such applications and their execution and monitoring in a heterogeneous environment consisting of a network of workstations, specialized machines, and parallel architectures.

We have been implementing a Java-based three-tier prototype system which supports a thin client interface for the design and execution of multi-module codes. The middle tier consists of logic to process the user input and also to manage the resource controllers which comprise the third tier. In the last few months we have focused on the issue of resource discovery and monitoring. In particular, we have implemented an add-on module to manage the resources based on the JINI technology developed by Sun for resource management. JINI allows independent resources to announce their presence and current status to a central server. This module provides a client interface which allows the user to monitor the current status of the resources. One of the issues with JINI is that it uses the multicast protocol for its discovery and join processes. Such protocols do not work over subnets or across domains. We have designed a hierarchical implementation of servers which allows the resources to announce their presence across the whole Arcade environment even if it spans multiple domains. Similarly, it allows the resource allocation module to query the status of resources across the whole environment.

We continue to develop the system adding other features such as support for conducting parameter studies. We also intend to expand the kind of modules that can be used by Arcade, in particular providing support for CORBA-based components.

This research was conducted in collaboration with K. Maly, A. Al-Theneyan, and M. Zubair (Old Dominion University).

### *Languages for High Performance and Distributed Computing*

There are many approaches to exploiting the power of parallel and distributed computers. Under this project, our focus is to evaluate these different approaches, proposing extensions and new compilation techniques where appropriate.

Recently a proposal was put forth for a set of language extensions to Fortran and C based upon a fork-join model of parallel execution; called OpenMP, it aims to provide a portable shared memory programming interface for shared memory and low latency systems. However, these extensions ignore the issue of data locality which becomes a performance issue on shared address space machines which use a physically distributed memory system. We have proposed a set of OpenMP extensions to allow users to express the distribution of the data structures in a manner similar to the one used in HPF. We are currently in the process of implementing these extensions in order to study their efficacy.

We have also continued our study on the applicability of HPF to a series of codes using semi-structured grids ranging from multiblock, semi-coarsening multigrid, and structured AMR algorithms. We have examined a range of data distribution strategies for these algorithms and have tried to characterize the situations under which each of these strategies would produce the best results.

OPUS, a language jointly developed by ICASE and University of Vienna, provides high-level support for programming multimodule applications. In the last few months we have redesigned and reimplemented the Opus runtime system. We have also completed the compiler front-end necessary for translating Opus programs to target the runtime system. This translator has been implemented using the Vienna Fortran Compiler System of the University of Vienna. The system allows users to translate and execute Opus programs across a network of workstations. We are in the process of evaluating our design and enhancing it to incorporate support for distributed processing within Opus modules.

This research was conducted in collaboration with B. Chapman (University of Houston), Erwin Laure (University of Vienna), and H. Zima (University of Vienna).

## ALEX POTHEN

### *Parallel Algorithms for Incomplete Factorization Preconditioners*

The parallel computation of incomplete factorization (ILU) preconditioners for solving large systems of equations has, until recently, remained an elusive goal. We propose to develop new algorithmic approaches that avoid the serial bottlenecks that have plagued existing algorithms, to implement these algorithms, and to identify applications where these preconditioners are effective.

The new algorithm is based on a characterization of the fill (zero elements in the coefficient matrix becoming nonzero during the factorization) in terms of paths in the adjacency graph associated with the coefficient matrix. We assume that the adjacency graph can be partitioned into subgraphs of roughly equal sizes such that few edges are cut by the partition. We map the subgraphs to processors, form a subdomain interconnection graph, and order the subdomains so as to reduce global dependences. On each subdomain, we locally reorder the interior vertices before the boundary vertices. This reordering limits the fill that joins a subgraph on one processor to a subgraph on another, and enhances the concurrency in the computation. The preconditioner computation takes places in two phases: in the first phase, each processor computes the rows of the preconditioner corresponding to the interior vertices of their subdomains. In the second phase, the rows corresponding to the boundary nodes are computed.

Our preliminary results on the SGI Origin show efficiencies greater than 75% on up to 16 processors. We are continuing to develop our parallel implementation, and are incorporating new algorithms that we have designed for efficient serial computation of preconditioners.

This research was conducted in collaboration with David Hysom (Old Dominion University and ICASE).

### *Spindle: An Algorithmic Laboratory for Ordering Algorithms*

We have begun to work on an algorithmic laboratory for quickly prototyping promising algorithms and experimenting with a collection of algorithmic variants for several ordering problems. Among these are the fill reduction problem: Order the rows and columns of the coefficient matrix to reduce the fill in sparse Gaussian elimination (both complete and incomplete factorizations); and the sequencing problem: Given a set of elements, and pairs of elements that are related, order the elements such that related elements are numbered consecutively. We employ object-oriented design techniques (OOD) to make the laboratory flexible and easy to extend.

OOD manages complexity by means of decomposition and abstraction. We decompose our software into two main types of objects: structural objects corresponding to data structures, and algorithmic objects corresponding to algorithms. This design decouples data structures from algorithms, permitting a user to

experiment with different algorithms and different data structures, and if necessary develop new algorithms and data structures. We have implemented seven variants from the family of minimum degree ordering algorithms using this design paradigm. Some of these algorithms were developed only in the past few years, and prior to our work, there was no single code that implemented all of these algorithms. Our implementation makes it possible for us to change ordering algorithms midstream while ordering a problem. We have found this to be of benefit, since a hybrid algorithm that employs the multiple minimum degree (MMD) algorithm and switches at later stages to the approximate minimum degree (AMD) algorithm can improve performance for problems where either algorithm has poor performance. These ordering algorithms are quite sophisticated, and their performance on various problem classes is poorly understood. Our algorithmic laboratory enhances our understanding of these issues since encapsulation makes it possible to examine the state of the objects in our code during execution.

We have also implemented wavefront-reducing algorithms—such as the Cuthill-McKee and Sloan ordering algorithms—in our library. Spindle, our code, is available as a stand-alone program and with an interface to Matlab.

This research was conducted in collaboration with Gary Kumfert (Old Dominion University and ICASE).

## KEVIN P. ROE

### *Parallelization of a Multigrid Incompressible Viscous Cavity Flow Solver Using OpenMP*

Effective use of parallel machines requires easily maintainable and portable programming models that allow users to exploit parallelism in applications written in a standard high-level language. MPI provides portability, however it can be more difficult to maintain and is not a high-level programming model. High Performance Fortran (HPF) is portable and fairly easy to maintain. OpenMP is also portable on shared memory architectures and fairly easy to maintain, although it can only be used on shared memory machines. OpenMP has some advantages over HPF and MPI when one is using a shared memory machine. Such as allowing the user to incrementally parallelize their code. Another benefit is that when the number of processors is changed that data residing in memory does not have to be reshaped.

To evaluate OpenMP's capabilities, we examine a two-dimensional multigrid incompressible viscous flow solver. This solver, originally written to be run sequentially, only required one major change. The Symmetric Gauss Seidel (SGS) algorithm that was originally used had to be replaced because its red-black parallel version was numerically unstable. Since we were more interested in testing OpenMP's capabilities, a simple parallel Jacobi algorithm was substituted in its place. Results of the code's parallelization using OpenMP on the SGI Origin2000 at NASA Ames were promising. Parallel efficiencies were in the 90-100% range for four processors on a problem size of 512x512. Tests using a different number of processors for each grid level at runtime were also conducted. We were able to reduce the overhead associated with using too many processors on a small problem size by specifying the number of threads (and hence processors) for each grid level at runtime.

We are still investigating where the loss in efficiency is occurring; we believe that larger problem sizes will yield better parallel efficiencies when more processors are utilized. We will also examine a mechanism for determining the ideal number of processors to utilize for each grid level at runtime.

This research was conducted in collaboration with Piyush Mehrotra (ICASE).

## LINDA STALS

### *Solution Techniques for Radiation Transport Equations*

When modeling radiation transport, a system of three nonlinear time-dependent equations is often used. Due to the behavior of the nonlinearities, this system is computationally expensive to solve. We are studying the use of two different approaches to reduce the solution time, namely, the use of better solution techniques, such as multigrid methods, and the use of parallel machines.

As a preliminary study of the radiation transport equations, we have considered the special case where all energies are in equilibrium. In such a case, the system of equations can be reduced to a single equation. This single equation is interesting in its own right as it contains strong nonlinearities and large jumps in the coefficients. The results and lessons learned in the study of this single equation will be used when we implement the system of three equations.

The discretization technique we used was the finite element method with piecewise linear basis elements. We are currently comparing our results with those obtained by other groups, which use different discretization techniques, to ensure that the finite element method is ‘capturing’ the right information.

We also compared the use of Newton’s method with the FAS (nonlinear multigrid) scheme. We found that when the jumps in the coefficients were not too large both methods performed well. However, when the size of the jumps was increased we needed to modify our algorithms. In particular, for the FAS scheme to work properly, the equation on the coarsest grid had to be solved to a high degree of accuracy. For Newton’s method, automatically calculating the step size greatly reduced the number of iterations. Furthermore, the use of adaptive refinement helped the solution process as the approximation calculated on the coarser grids gave a good initial guess to the solution on the current grid. As the system of three equations also contains large jumps in the coefficients, we believe that the techniques and methods which we have shown to work here will be a good starting point when we try to solve the system.

We ran the code on a network of workstations and verified that we get the same mathematical results as though it were run in parallel. However, we do not have any parallel efficiency results yet. One of our next goals is to test the parallel efficiency of our approach.

The form of the nonlinear term in radiation transport equations can vary. So far we have only considered the weakest or least nonlinear form. We would also like to rerun our experiments using the other forms of the equations.

This research was conducted in collaboration with David Keyes and Alex Pothen (Old Dominion University and ICASE) and Dimitri Mavriplis (ICASE) as part of an ASCI project.

## HANS ZIMA

### *Feedback-directed and Adaptive Compilation*

Traditionally, compilation has been seen as a batch process, in which a high-level language is translated into a machine or assembly language executable on a given target machine. Compilation is performed in a given machine/system environment known to the compiler, which can be exploited for optimizing the target program. If the environment is not known at compilation time, or if it may change during execution, the target program has to be parameterized accordingly. The late binding associated with such a parameterization guarantees flexibility on the one hand, but on the other hand may result in less efficient code if compared to an early binding approach. The objective of this study is to examine the changing role of the compiler in modern computing environments and its interrelationship with performance tools.

The traditional view of compilation can no longer be maintained, for reasons due to the evolution of computing systems, languages, and compiling techniques. For example, in a heterogeneous environment (which may encompass the whole Internet), a client may send a source program (or a partially translated intermediate version of the source) to a remote server for compilation and execution. Similarly, in contrast to traditional static compilation, the Java HotSpot virtual machine identifies bottlenecks during interpretation of a Java program, and optimizes execution by performing on-the-fly compilation to native code. The *inspector/executor* approach, which is being routinely used for the runtime optimization of parallel loops in high-level languages, is an example for runtime compilation using feedback based on information gained during execution. Systems such as *ATLAS* and *FFTW* use performance feedback to optimize the code for a given environment. A number of programming systems (such as the AURORA Compilation Environment) use performance feedback from execution traces for performance tuning in the compile/execute cycle.

We are currently developing a taxonomy of the existing approaches in this field. Following this, we will study the possibility of extending the Vienna Fortran Compilation system and related performance tools to demonstrate proof-of-concept solutions for relevant application problems.

This research was conducted in collaboration with Piyush Mehrotra (ICASE).

## REPORTS AND ABSTRACTS

Sidilkover, David: *A new time-space accurate scheme for hyperbolic problems I: Quasi-explicit case.* ICASE Report No. 98-25, (NASA/CR-1998-208436), October 27, 1998, 24 pages. Submitted to Communications in Applied Analysis.

This paper presents a new discretization scheme for hyperbolic systems of conservations laws. It satisfies the TVD property and relies on the new high-resolution mechanism which is compatible with the genuinely multidimensional approach proposed recently. This work can be regarded as a first step towards extending the genuinely multidimensional approach to unsteady problems. Discontinuity capturing capabilities and accuracy of the scheme are verified by a set of numerical tests.

Mavriplis, Dimitri J.: *On convergence acceleration techniques for unstructured meshes.* ICASE Report No. 98-44, (NASA/CR-1998-208732), November 2, 1998, 35 pages.

A discussion of convergence acceleration techniques as they relate to computational fluid dynamics problems on unstructured meshes is given. Rather than providing a detailed description of particular methods, the various different building blocks of current solution techniques are discussed and examples of solution strategies using one or several of these ideas are given. Issues relating to unstructured grid CFD problems are given additional consideration, including suitability of algorithms to current hardware trends, memory and cpu tradeoffs, treatment of nonlinearities, and the development of efficient strategies for handling anisotropy-induced stiffness. The outlook for future potential improvements is also discussed.

Povitsky, A.: *Parallel directionally split solver based on reformulation of pipelined Thomas algorithm.* ICASE Report No. 98-45, (NASA/CR-1998-208733), October 27, 1998, 30 pages. To be submitted to SIAM Journal of Scientific Computing.

In this research an efficient parallel algorithm for 3-D directionally split problems is developed. The proposed algorithm is based on a reformulated version of the pipelined Thomas algorithm that starts the backward step computations immediately after the completion of the forward step computations for the first portion of lines. This algorithm has data available for other computational tasks while processors are idle from the Thomas algorithm.

The proposed 3-D directionally split solver is based on the static scheduling of processors where local and non-local, data-dependent and data-independent computations are scheduled while processors are idle. A theoretical model of parallelization efficiency is used to define optimal parameters of the algorithm, to show an asymptotic parallelization penalty and to obtain an optimal cover of a global domain with subdomains.

It is shown by computational experiments and by the theoretical model that the proposed algorithm reduces the parallelization penalty about two times over the basic algorithm for the range of the number of processors (subdomains) considered and the number of grid nodes per subdomain.



Chow, P.L., and L. Maestrello: *Vibrational control of a nonlinear elastic panel*. ICASE Report No. 98-46, (NASA/CR-1998-208734), November 5, 1998, 19 pages. To be submitted to the Journal of the Acoustic Society of America.

The paper is concerned with the stabilization of the nonlinear panel oscillation by an active control. The control is actuated by a combination of additive and parametric vibrational forces. A general method of vibrational control is presented for stabilizing panel vibration satisfying a nonlinear beam equation. To obtain analytical results, a perturbation technique is used in the case of weak nonlinearity. Possible application to the other type of problems is briefly discussed.

Booker, Andrew J., J.E. Dennis, Jr., Paul D. Frank, David B. Serafini, Virginia Torczon, and Michael W. Trosset: *A rigorous framework for optimization of expensive functions by surrogates*. ICASE Report No. 98-47, (NASA/CR-1998-208735), November 5, 1998, 24 pages. To appear in Structural Optimization.

The goal of the research reported here is to develop rigorous optimization algorithms to apply to some engineering design problems for which design application of traditional optimization approaches is not practical. This paper presents and analyzes a framework for generating a sequence of approximations to the objective function and managing the use of these approximations as surrogates for optimization. The result is to obtain convergence to a minimizer of an expensive objective function subject to simple constraints. The approach is widely applicable because it does not require, or even explicitly approximate, derivatives of the objective. Numerical results are presented for a 31-variable helicopter rotor blade design example and for a standard optimization test example.

Povitsky, A.: *Parallelization of the pipelined Thomas algorithm*. ICASE Report No. 98-48, (NASA/CR-1998-208736), December 3, 1998, 26 pages. Submitted to the Journal of Parallel and Distributed Computing.

In this study the following questions are addressed. Is it possible to improve the parallelization efficiency of the Thomas algorithm? How should the Thomas algorithm be formulated in order to get solved lines that are used as data for other computational tasks while processors are idle?

To answer these questions, two-step pipelined algorithms (PAs) are introduced formally. It is shown that the idle processor time is invariant with respect to the order of backward and forward steps in PAs starting from one outermost processor. The advantage of PAs starting from two outermost processors is small. Versions of the pipelined Thomas algorithms considered here fall into the category of PAs.

These results show that the parallelization efficiency of the Thomas algorithm cannot be improved directly. However, the processor idle time can be used if some data has been computed by the time processors become idle. To achieve this goal the Immediate Backward pipelined Thomas Algorithm (IB-PTA) is developed in this article. The backward step is computed immediately after the forward step has been completed for the first portion of lines. This enables the completion of the Thomas algorithm for some of these lines before processors become idle. An algorithm for generating a static processor schedule recursively is developed. This schedule is used to switch between forward and backward computations and to control communications between processors. The advantage of the IB-PTA over the basic PTA is the presence of solved lines, which are available for other computations, by the time processors become idle.

Rubinstein, Robert, and Ye Zhou: *Effects of helicity on Lagrangian and Eulerian time correlations in turbulence*. ICASE Report No. 98-49, (NASA/CR-1998-208737), November 5, 1998, 10 pages. Submitted to Physics of Fluids.

Taylor series expansions of turbulent time correlation functions are applied to show that helicity influences Eulerian time correlations more strongly than Lagrangian time correlations: to second order in time, the helicity effect on Lagrangian time correlations vanishes, but the helicity effect on Eulerian time correlations is nonzero. Fourier analysis shows that the helicity effect on Eulerian time correlations is confined to the largest inertial range scales. Some implications for sound radiation by swirling flows are discussed.

Abarbanel, Saul, Adi Ditkowski, and Amir Yefet: *Bounded error schemes for the wave equation on complex domains*. ICASE Report No. 98-50, (NASA/CR-1998-208740), November 20, 1998, 17 pages. Submitted to IEEE Trans. Antennas Propagat.

This paper considers the application of the method of boundary penalty terms ("SAT") to the numerical solution of the wave equation on complex shapes with Dirichlet boundary conditions. A theory is developed, in a semi-discrete setting, that allows the use of a Cartesian grid on complex geometries, yet maintains the order of accuracy with only a linear temporal error-bound. A numerical example, involving the solution of Maxwell's equations inside a 2-D circular wave-guide demonstrates the efficacy of this method in comparison to others (e.g., the staggered Yee scheme) - we achieve a decrease of two orders of magnitude in the level of the  $L_2$ -error.

Darmofal, David: *Eigenmode analysis of boundary conditions for the one-dimensional preconditioned Euler equations*. ICASE Report No. 98-51, (NASA/CR-1998-208741), November 20, 1998, 15 pages. To be submitted to AIAA 1999 CFD Conference and SIAM Journal of Numerical Analysis.

An analysis of the effect of local preconditioning on boundary conditions for the subsonic, one-dimensional Euler equations is presented. Decay rates for the eigenmodes of the initial boundary value problem are determined for different boundary conditions. Riemann invariant boundary conditions based on the unpreconditioned Euler equations are shown to be reflective with preconditioning, and, at low Mach numbers, disturbances do not decay. Other boundary conditions are investigated which are non-reflective with preconditioning and numerical results are presented confirming the analysis.

Tsynkov, Semyon, Saul Abarbanel, Jan Nordstrom, Viktor Ryaben'kii, and Veer Vatsa: *Global artificial boundary conditions for computation of external flow problems with propulsive jets*. ICASE Report No. 98-52, (NASA/CR-1998-208746), December 3, 1998, 25 pages. Submitted to the 14th AIAA CFD Conference.

We propose new global artificial boundary conditions (ABC's) for computation of flows with propulsive jets. The algorithm is based on application of the difference potentials method (DPM). Previously, similar boundary conditions have been implemented for calculation of external compressible viscous flows around finite bodies. The proposed modification substantially extends the applicability range of the DPM-based algorithm. In the paper, we present the general formulation of the problem, describe our numerical methodology, and discuss the corresponding computational results. The particular configuration that we analyze is a slender three-dimensional body with boat-tail geometry and supersonic jet exhaust in a subsonic external flow under zero angle of attack. Similarly to the results obtained earlier for the flows around airfoils and

wings, current results for the jet flow case corroborate the superiority of the DPM-based ABC's over standard local methodologies from the standpoints of accuracy, overall numerical performance, and robustness.

Xu, Kun: *Gas-kinetic theory based flux splitting method for ideal magnetohydrodynamics*. ICASE Report No. 98-53, (NASA/1998-208747), December 3, 1998, 22 pages. To be submitted to the Journal of Computational Physics.

A gas-kinetic solver is developed for the ideal magnetohydrodynamics (MHD) equations. The new scheme is based on the direct splitting of the flux function of the MHD equations with the inclusion of "particle" collisions in the transport process. Consequently, the artificial dissipation in the new scheme is much reduced in comparison with the MHD Flux Vector Splitting Scheme. At the same time, the new scheme is compared with the well-developed Roe-type MHD solver. It is concluded that the kinetic MHD scheme is more robust and efficient than the Roe-type method, and the accuracy is competitive. In this paper the general principle of splitting the macroscopic flux function based on the gas-kinetic theory is presented. The flux construction strategy may shed some light on the possible modification of AUSM- and CUSP-type schemes for the compressible Euler equations, as well as to the development of new schemes for a non-strictly hyperbolic system.

Holt, Maurice: *3D characteristics*. ICASE Report No. 98-54, (NASA/CR-1998-208958), December 23, 1998, 10 pages. Submitted to Springer Series in Computational Physics.

Contributions to the Method of Characteristics in Three Dimensions, which previously received incomplete recognition, are reviewed. They mostly follow from a fundamental paper by Rusanov which led to several developments in Russia, described by Chushkin.

Lian, Yongsheng, and Kun Xu: *A gas-kinetic scheme for reactive flows*. ICASE Report No. 98-55, (NASA/CR-1998-208963), December 23, 1998, 16 pages. To be submitted to Computers and Fluids.

In this paper, the gas-kinetic BGK scheme for the compressible flow equations is extended to chemical reactive flow. The mass fraction of the unburnt gas is implemented into the gas kinetic equation by assigning a new internal degree of freedom to the particle distribution function. The new variable can be also used to describe fluid trajectory for the nonreactive flows. Due to the gas-kinetic BGK model, the current scheme basically solves the Navier-Stokes chemical reactive flow equations. Numerical tests validate the accuracy and robustness of the current kinetic method.

Xu, Kun, and Shiu-Hong Lui: *Rayleigh-Bénard simulation using gas-kinetic BGK scheme in the incompressible limit*. ICASE Report No. 98-56, (NASA/CR-1998-208964), December 23, 1998, 19 pages. Submitted to Physical Review E.

In this paper, a gas-kinetic BGK model is constructed for the Rayleigh-Bénard thermal convection in the incompressible flow limit, where the flow field and temperature field are described by two coupled BGK models. Since the collision times and pseudo-temperature in the corresponding BGK models can be different, the Prandtl number can be changed to any value instead of a fixed  $Pr=1$  in the original BGK model. The 2D Rayleigh-Bénard thermal convection is studied and numerical results are compared with theoretical ones as well as other simulation results.

Lewis, Robert Michael, Virginia Torczon, and Michael W. Trosset: *Why pattern search works*. ICASE Report No. 98-57, (NASA/CR-1998-208966), December 23, 1998, 17 pages. To appear in Optima, The Mathematical Programming Society Newsletter.

Pattern search methods are a class of direct search methods for nonlinear optimization. Since the introduction of the original pattern search methods in the late 1950s and early 1960s, they have remained popular with users due to their simplicity and the fact that they work well in practice on a variety of problems. More recently, the fact that they are provably convergent has generated renewed interest in the nonlinear programming community. The purpose of this article is to describe what pattern search methods are and why they work.

Kumfert, Gary, and Alex Pothén: *An object-oriented collection of minimum degree algorithms: Design, implementation, and experiences*. ICASE Report No. 99-1, (NASA/CR-1999-208977), January 29, 1999, 15 pages. In Computing in Object-oriented Parallel Environments, Lecture Notes in Computer Science 1505.

The multiple minimum degree (MMD) algorithm and its variants have enjoyed 20+ years of research and progress in generating fill-reducing orderings for sparse, symmetric positive definite matrices. Although conceptually simple, efficient implementations of these algorithms are deceptively complex and highly specialized.

In this case study, we present an object-oriented library that implements several recent minimum degree-like algorithms. We discuss how object-oriented design forces us to decompose these algorithms in a different manner than earlier codes and demonstrate how this impacts the flexibility and efficiency of our C++ implementation. We compare the performance of our code against other implementations in C or Fortran.

Dobrian, Florin, Gary Kumfert, and Alex Pothén: *Object-oriented design for sparse direct solvers*. ICASE Report No. 99-2, (NASA/CR-1999-208978), January 20, 1999, 12 pages. In Computing in Object-oriented Parallel Environments, Lecture Notes in Computer Science 1505.

We discuss the object-oriented design of a software package for solving sparse, symmetric systems of equations (positive definite and indefinite) by direct methods. At the highest layers, we decouple data structure classes from algorithmic classes for flexibility. We describe the important structural and algorithmic classes in our design, and discuss the trade-offs we made for high performance. The kernels at the lower layers were optimized by hand. Our results show no performance loss from our object-oriented design, while providing flexibility, ease of use, and extensibility over solvers using procedural design.

Cleaveland, Rance, Gerald Lüttgen, and V. Natarajan: *Priority in process algebras*. ICASE Report No. 99-3, (NASA/CR-1999-208979), January 25, 1999, 48 pages. To appear in Handbook of Process Algebras.

This paper surveys the semantic ramifications of extending traditional process algebras with notions of priority that allow for some transitions to be given precedence over others. These enriched formalisms allow one to model system features such as interrupts, prioritized choice, or real-time behavior.

Approaches to priority in process algebras can be classified according to whether the induced notion of pre-emption on transitions is global or local and whether priorities are static or dynamic. Early work in the area concentrated on global pre-emption and static priorities and led to formalisms for modeling interrupts and aspects of real-time, such as maximal progress, in centralized computing environments. More recent

research has investigated localized notions of pre-emption in which the distribution of systems is taken into account, as well as dynamic priority approaches, i.e., those where priority values may change as systems evolve. The latter allows one to model behavioral phenomena such as scheduling algorithms and also enables the efficient encoding of real-time semantics.

Technically, this paper studies the different models of priorities by presenting extensions of Milner's Calculus of Communicating Systems (CCS) with static and dynamic priority as well as with notions of global and local pre-emption. In each case the operational semantics of CCS is modified appropriately, behavioral theories based on strong and weak bisimulation are given, and related approaches for different process-algebraic settings are discussed.

Lüttgen, Gerald, Girish Bhat, and Rance Cleaveland: *A practical approach to implementing real-time semantics*. ICASE Report No. 99-4, (NASA/CR-1999-208980), January 25, 1999, 33 pages. To appear in *Annals of Software Engineering*.

This paper investigates implementations of process algebras which are suitable for modeling concurrent real-time systems. It suggests an approach for efficiently implementing real-time semantics using dynamic priorities. For this purpose a process algebra with dynamic priority is defined, whose semantics corresponds one-to-one to traditional real-time semantics. The advantage of the dynamic-priority approach is that it drastically reduces the state-space sizes of the systems in question while preserving all properties of their functional and real-time behavior.

The utility of the technique is demonstrated by a case study which deals with the formal modeling and verification of the SCSI-2 bus-protocol. The case study is carried out in the Concurrency Workbench of North Carolina, an automated verification tool in which the process algebra with dynamic priority is implemented. It turns out that the state space of the bus-protocol model is about an order of magnitude smaller than the one resulting from real-time semantics. The accuracy of the model is proved by applying model checking for verifying several mandatory properties of the bus protocol.

Lui, ShiuHong, and Kun Xu: *Entropy analysis of kinetic flux vector splitting schemes for the compressible Euler equations*. ICASE Report No. 99-5, (NASA/CR-1999-208981), January 29, 1999, 18 pages.

Flux Vector Splitting (FVS) scheme is one group of approximate Riemann solvers for the compressible Euler equations. In this paper, the discretized entropy condition of the Kinetic Flux Vector Splitting (KFVS) scheme based on the gas-kinetic theory is proved. The proof of the entropy condition involves the entropy definition difference between the distinguishable and indistinguishable particles.

Xu, Kun: *Gas evolution dynamics in Godunov-type schemes and analysis of numerical shock instability*. ICASE Report No. 99-6, (NASA/CR-1999-208985), January 28, 1999, 21 pages. To be submitted to the *International Journal of Numerical Methods in Fluids*.

In this paper we are going to study the gas evolution dynamics of the exact and approximate Riemann solvers, e.g., the Flux Vector Splitting (FVS) and the Flux Difference Splitting (FDS) schemes. Since the FVS scheme and the Kinetic Flux Vector Splitting (KFVS) scheme have the same physical mechanism and similar flux function, based on the analysis of the discretized KFVS scheme the weakness and advantage of the FVS scheme are closely observed. The subtle dissipative mechanism of the Godunov method in the 2D

case is also analyzed, and the physical reason for shock instability, i.e., carbuncle phenomena and odd-even decoupling, is presented.

Rubinstein, Robert: *Double resonance and spectral scaling in the weak turbulence theory of rotating and stratified turbulence*. ICASE Report No. 99-7, (NASA/CR-1999-208996), February 5, 1999, 19 pages. Submitted to Physical Review E.

In rotating turbulence, stably stratified turbulence, and in rotating stratified turbulence, heuristic arguments concerning the turbulent time scale suggest that the inertial range energy spectrum scales as  $k^{-2}$ . From the viewpoint of weak turbulence theory, there are three possibilities which might invalidate these arguments: four-wave interactions could dominate three-wave interactions leading to a modified inertial range energy balance, double resonances could alter the time scale, and the energy flux integral might not converge. It is shown that although double resonances exist in all of these problems, they do not influence overall energy transfer. However, the resonance conditions cause the flux integral for rotating turbulence to diverge logarithmically when evaluated for a  $k^{-2}$  energy spectrum; therefore, this spectrum requires logarithmic corrections. Finally, the role of four-wave interactions is briefly discussed.

Rubinstein, Robert, and Ye Zhou: *The dissipation range in rotating turbulence*. ICASE Report No. 99-8, (NASA/CR-1999-208997), February 5, 1999, 11 pages. Submitted to Physical Review E.

The dissipation range energy balance of the direct interaction approximation is applied to rotating turbulence when rotation effects persist well into the dissipation range. Assuming that  $RoRe^{1/2} \ll 1$  and that three-wave interactions are dominant, the dissipation range is found to be concentrated in the wavevector plane perpendicular to the rotation axis. This conclusion is consistent with previous analyses of inertial range energy transfer in rotating turbulence, which predict the accumulation of energy in those scales.

Mavriplis, Dimitri J., and S. Pirzadeh: *Large-scale parallel unstructured mesh computations for 3D high-lift analysis*. ICASE Report No. 99-9, (NASA/CR-1999-208999), February 11, 1999, 26 pages. Submitted to AIAA Journal of Aircraft.

A complete “geometry to drag-polar” analysis capability for the three-dimensional high-lift configurations is described. The approach is based on the use of unstructured meshes in order to enable rapid turnaround for complicated geometries that arise in high-lift configurations. Special attention is devoted to creating a capability for enabling analyses on highly resolved grids. Unstructured meshes of several million vertices are initially generated on a work-station, and subsequently refined on a supercomputer. The flow is solved on these refined meshes on large parallel computers using an unstructured agglomeration multigrid algorithm. Good prediction of lift and drag throughout the range of incidences is demonstrated on a transport take-off configuration using up to 24.7 million grid points. The feasibility of using this approach in a production environment on existing parallel machines is demonstrated, as well as the scalability of the solver on machines using up to 1450 processors.

Xu, Kun, and Li-Shi Luo: *Connection between the lattice Boltzmann equation and the beam scheme*. ICASE Report No. 99-10, (NASA/CR-1999-209001), February 12, 1999, 14 pages. Submitted to Physical Review E.

In this paper we analyze and compare the lattice Boltzmann equation with the beam scheme in details. We notice the similarity and differences between the lattice Boltzmann equation and the beam scheme. We show that the accuracy of the lattice Boltzmann equation is indeed second order in space. We discuss the advantages and limitations of lattice Boltzmann equation and the beam scheme. Based on our analysis, we propose an improved multi-dimensional beam scheme.

Baggag, Abdelkader, Harold Atkins, Can Özturan, and David Keyes: *Parallelization of an object-oriented unstructured aeroacoustics solver*. ICASE Report No. 99-11, (NASA/CR-1999-209098), February 16, 1999, 16 pages. Submitted to the Proceedings of the 9th SIAM Conference on Parallel Processing for Scientific Computing.

A computational aeroacoustics code based on the discontinuous Galerkin method is ported to several parallel platforms using MPI. The discontinuous Galerkin method is a compact high-order method that retains its accuracy and robustness on non-smooth unstructured meshes. In its semi-discrete form, the discontinuous Galerkin method can be combined with explicit time marching methods making it well suited to time accurate computations. The compact nature of the discontinuous Galerkin method also makes it well suited for distributed memory parallel platforms. The original serial code was written using an object-oriented approach and was previously optimized for cache-based machines. The port to parallel platforms was achieved simply by treating partition boundaries as a type of boundary condition. Code modifications were minimal because boundary conditions were abstractions in the original program. Scalability results are presented for the SGI Origin, IBM SP2, and clusters of SGI and Sun workstations. Slightly superlinear speedup is achieved on a fixed-size problem on the Origin, due to cache effects.

Arian, E., A. Batterman, and E.W. Sachs: *Approximation of the Newton step by a defect correction process*. ICASE Report No. 99-12, (NASA/CR-1999-209099), February 16, 1999, 35 pages. To be submitted to SIAM Journal of Optimization.

In this paper, an optimal control problem governed by a partial differential equation is considered. The Newton step for this system can be computed by solving a coupled system of equations. To do this efficiently with an iterative defect correction process, a modifying operator is introduced into the system. This operator is motivated by local mode analysis. The operator can be used also for preconditioning in GMRES. We give a detailed convergence analysis for the defect correction process and show the derivation of the modifying operator. Numerical tests are done on the small disturbance shape optimization problem in two dimensions for the defect correction process and for GMRES.

Rubinstein, Robert, and Aaron H. Auslender: *Relaxation from steady states far from equilibrium and the persistence of anomalous shock behavior in weakly ionized gases*. ICASE Report No. 99-13, (NASA/CR-1999-209105), March 3, 1999, 13 pages. To be submitted to Physical Review E.

The decay of anomalous effects on shock waves in weakly ionized gases following plasma generator extinction has been measured in the anticipation that the decay time must correlate well with the relaxation

time of the mechanism responsible for the anomalous effects. When the relaxation times cannot be measured directly, they are inferred theoretically, usually assuming that the initial state is nearly in thermal equilibrium. In this paper, it is demonstrated that relaxation from any steady state far from equilibrium, including the state of a weakly ionized gas, can proceed much more slowly than arguments based on relaxation from near equilibrium states might suggest. This result justifies a more careful analysis of the relaxation times in weakly ionized gases and suggests that although the experimental measurements of relaxation times did not lead to an unambiguous conclusion, this approach to understanding the anomalous effects may warrant further investigation.

Diskin, Boris, and James L. Thomas: *Solving upwind-biased discretizations: Defect-correction iterations*. ICASE Report No. 99-14, (NASA/CR-1999-209106), March 3, 1999, 27 pages. To be submitted to the SIAM Journal of Scientific Computing.

This paper considers defect-correction solvers for a second order upwind-biased discretization of the 2D convection equation. The following important features are reported

1. The asymptotic convergence rate is about 0.5 per defect-correction iteration.
2. If the operators involved in defect-correction iterations have different approximation order, then the initial convergence rates may be very slow. The number of iterations required to get into the asymptotic convergence regime might grow on fine grids as a negative power of  $h$ . In the case of a second order target operator and a first order driver operator, this number of iterations is roughly proportional to  $h^{-1/3}$ .
3. If both the operators have the second approximation order, the defect-correction solver demonstrates the asymptotic convergence rate after three iterations at most. The same three iterations are required to converge algebraic error below the truncation error level.

A novel comprehensive half-space Fourier mode analysis (which, by the way, can take into account the influence of discretized outflow boundary conditions as well) for the defect-correction method is developed. This analysis explains many phenomena observed in solving non-elliptic equations and provides a close prediction of the actual solution behavior. It predicts the convergence rate for each iteration and the asymptotic convergence rate. As a result of this analysis, a new very efficient adaptive multigrid algorithm solving the discrete problem to within a given accuracy is proposed. Numerical simulations confirm the accuracy of the analysis and the efficiency of the proposed algorithm. The results of the numerical tests are reported.



## INTERIM REPORTS

Bokhari, Shahid H., and Dimitri J. Mavriplis: *The Tera multithreaded architecture and unstructured meshes*. ICASE Interim Report No. 33, (NASA/CR-1998-208953), December 11, 1998, 23 pages.

The Tera Multithreaded Architecture (MTA) is a new parallel supercomputer currently being installed at San Diego Supercomputing Center (SDSC). This machine has an architecture quite different from contemporary parallel machines. The computational processor is a custom design and the machine uses hardware to support very fine grained multithreading. The main memory is shared, hardware randomized and flat. These features make the machine highly suited to the execution of unstructured mesh problems, which are difficult to parallelize on other architectures.

We report the results of a study carried out during July-August 1998 to evaluate the execution of EUL3D, a code that solves the Euler equations on an unstructured mesh, on the 2 processor Tera MTA at SDSC.

Our investigation shows that parallelization of an unstructured code is extremely easy on the Tera. We were able to get an existing parallel code (designed for a shared memory machine), running on the Tera by changing only the compiler directives. Furthermore, a *serial* version of this code was compiled to run in parallel on the Tera by judicious use of directives to invoke the “full/empty” tag bits of the machine to obtain synchronization. This version achieves 212 and 406 Mflop/s on one and two processors respectively, and requires no attention to partitioning or placement of data—issues that would be of paramount importance in other parallel architectures.

Yefet, A., and E. Turkel: *Construction of three dimensional solutions for the Maxwell equations*. ICASE Interim Report No. 34, (NASA/CR-1998-208954), December 11, 1998, 10 pages.

We consider numerical solutions for the three dimensional time dependent Maxwell equations. We construct a fourth order accurate compact implicit scheme and compare it to the Yee scheme for free space in a box.

Trosset, Michael W.: *The Krigifier: A procedure for generating pseudorandom nonlinear objective functions for computational experimentation*. ICASE Interim Report No. 35, (NASA/CR-1999-209000), February 11, 1999, 11 pages.

Comprehensive computational experiments to assess the performance of algorithms for numerical optimization require (among other things) a practical procedure for generating pseudorandom nonlinear objective functions. We propose a procedure that is based on the convenient fiction that objective functions are realizations of stochastic processes. This report details the calculations necessary to implement our procedure for the case of certain stationary Gaussian processes and presents a specific implementation in the statistical programming language S-PLUS.

**ICASE COLLOQUIA**  
**October 1, 1998 – March 31, 1999**

<b>Name/Affiliation/Title</b>	<b>Date</b>
Cleaveland, Rance, State University of New York at Stony Brook "An Operational Semantics of Temporal Logic"	October 1
Ewins, David, Imperial College of Science, Technology & Medicine, London, UK "Modal Testing on the Move"	October 19
Bartz, Dirk, University of Tuebingen, Germany "Constructing Recursive Tree Hierarchies in Parallel"	October 26
Ho, Chih-Ming, University of California, Los Angeles "M3 System for Aerodynamic Control"	October 26
Huettner, Tobias, University of Tuebingen, Germany "High-resolution Textures"	October 26
Morris, Kirsten, University of Waterloo, Canada "Achievable Noise Reduction in Ducts"	November 9
Simpson, Robert W., Massachusetts Institute of Technology "The Problems of Quantifying Safety in Aviation"	November 10
Davies, Roger, University of Arizona "Progress Towards a Panorama of Cloud Reflectivity"	November 19
Shapiro, Gerald, Logistics Management Institute, McLean, VA "Modeling the Safety Implications of Aviation Operations"	November 19
Barnett, Arnold, Massachusetts Institute of Technology "Aviation Safety in Numbers"	November 23
Stathopoulos, Andreas, The College of William & Mary "Restarting Techniques for Arnoldi-like Eigenvalue Methods"	November 23
Curkendall, David, Jet Propulsion Laboratory "Data Visualization Corridors and the Digital Earth"	December 2

<b>Name/Affiliation/Title</b>	<b>Date</b>
Stals, Linda, Old Dominion University “Parallel Implementation of Multigrid Methods on Unstructured Grids”	December 11
Beck, Richard, Miami University, Oxford, OH “Gateway to the Future: OhioView Pilot: Test-bed for a National Space-based Geospatial Information Network”	January 8
Hart, Roger, ICASE “Applications of Laser-induced Thermal Acoustics to Flow Characterization”	January 13
Munoz, Cesar, SRI International, Menlo Park, CA “Types for Software Development”	January 19
Mascagni, Michael, University of Southern Mississippi “A Deterministic Particle Method for One-dimensional Reaction-diffusion Equations”	January 22
Lin, Huimin, Chinese Academy of Sciences “The ‘Symbolic’ Approach to Message-passing Processes”	January 25
Sobieski, Jaroslaw, NASA Langley Research Center “Compute as Fast as Engineers Can Think”	January 28
Sidilkover, David, ICASE “Towards a Unified Approach for Numerical Treatment of Incompressible and Compressible Steady Flow”	January 29
Rubinstein, Robert, ICASE “Characterization of Sound Radiation by Unresolved Scales of Motion in Computational Aeroacoustics”	February 10
Nikolaidis, Efstratios, Virginia Polytechnic Institute and State University “Design Under Uncertainty”	February 12
Botts, Mike, Global Hydrology and Climate Center, University of Alabama in Huntsville “Development and Application of the Java-based Space-time Toolkit for Integration of Disparate GeoSpatial Dynamic Data”	February 25
Ristorcelli, Raymond, Los Alamos National Laboratory “Lagrangian Covariance Analysis of Homogeneous Beta-plane Turbulence”	March 10

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